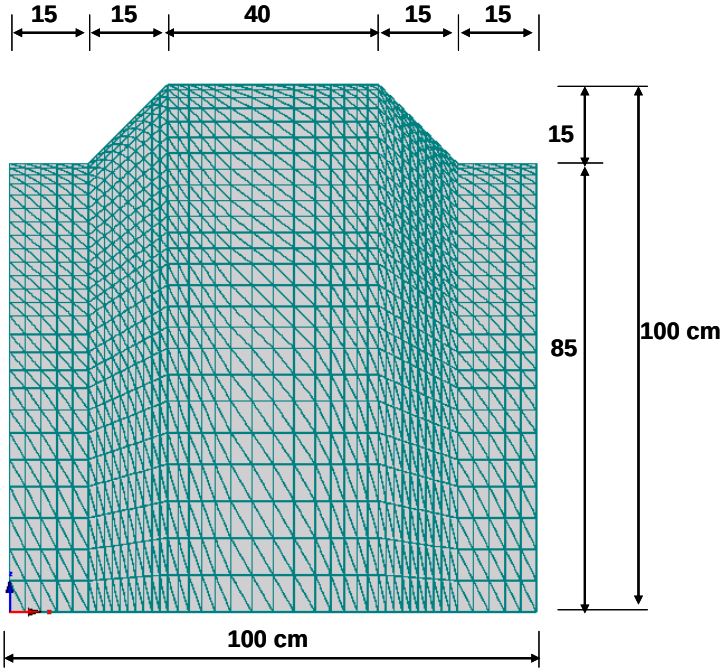
Unsatchem Tutorial: Furrow infiltration

A furrow irrigation problem is used in this tutorial to simulate two-dimensional infiltration of gypsum saturated water into a sodic soil. The simulation of sodic soil reclamation demonstrates the cation exchange feature of the UNSATCHEM module. The schematic representation of the flow domain for the considered furrow irrigation together with the finite element mesh is presented below. Several variants (such as using different irrigation water, effects of solution composition on hydraulic conductivity, etc) of the basic simulations (done first) are discussed in the second part of the tutorial.



Schematic representation and finite element mesh of the flow domain for the furrow irrigation system.

It is assumed that every other furrow is flooded with water and that the water level in the irrigated furrow is kept constant at a level of 6 cm. Due to symmetry, it is necessary to carry out the simulation only for the domain between the axis of two neighboring furrows. Free drainage is used as the bottom boundary condition and zero flux is considered on the rest of the boundary. The initial pressure head condition is -200 cm and the soil hydraulic properties of silt are used. Water infiltration is evaluated for 5 days.

The calculation is run at a constant temperature of 25 ^{o}C and a CO_2 concentration of 0.01 cm^3cm^{-3}. Root water uptake and evaporation were neglected. The bulk density of the soil was taken as 1.4 g cm^{-3} and molecular diffusion as 2 cm^2day^{-1}. Longitudinal and transverse dispersivities were equal to 2 and 0.2 cm, respectively.

The solution composition of the water initially present in the soil profile is that of the following highly sodic water: Ca_T=0.2, Mg_T=0.0, Na_T=4.8, K_T=0.0, Cl_T=4.6, SO_{4T}=0.0, Alk=0.4 $mmol_cL^{-1}$. The cation exchange capacity is equal to 100 $mmol_ckg^{-1}$ and is divided between exchangeable

calcium and sodium (a=5.0, a=95.0 $mmol_c kg^{-1}$). The following Gapon selectivity coefficients were used: $K_{Ca/Mg}$=0.896, $K_{Ca/Na}$=1.158, and $K_{Ca/k}$=0.111. The solution composition of the irrigation water was almost gypsum saturated: Ca_T=32.6, Mg_T=0.0, Na_T=4.8, K_T=0.0, Cl_T=5.0, SO_{4T}=32.0, Alk=0.4 $mmol_c L^{-1}$. As a consequence of the reactions of the irrigation water with the exchanger composition, cation exchange was the dominant chemical processes in the soil profile. Cation exchange is treated as an instantaneous process in the model.

Users become in this example familiar with the basic concept of the transport domain design (using simple geometry) and of chemical compositions used in the UNSATCHEM module. Initial and boundary conditions are specified, and graphical displays of the results using contour and spectrum maps, including animation, are provided, for a more complex transport domain than in the previous example.

Project Manager (File->Project Manager)
Button "New"

New Project (or File->New Project)
Name: UnsatchemFurrow
Description: Furrow irrigation with a solute pulse - Tutorial
Working Directory: Temporary – exists only when the project is open
Button "Next"

Domain Type and Units (Edit->Domain Geometry->Domain Type and Units)
Type of Geometry: 2D - Simple
2D-Domain Options: 2D - Vertical Plane XZ
Units: cm
Note that "Edit domain properties, initial and boundary conditions on geometric objects" is disabled. This approach can be used on with 2D-General Geometries.
Initial Workspace: X-Min=0, X-Max=100, Z-Min=0, Z-Max=100 cm (exact size of the transport domain)
Button "Next"

Rectangular Domain Definition (Edit->Domain Geometry->Simple Domain)
Lx: 100 cm
Lz: 100 cm
Slope α: 0
Button "Next"

Main Processes (Edit->Flow and Transport Parameters->Main Processes)
Check Boxes: Water Flow, Solute Transport, and Major Ion Chemistry
Button "Next"

Time Information (Edit->Flow and Transport Parameters->Time Information)
Time Units: days

Final Time: 5
Initial Time Step: 0.0001
Minimum Time Step: 0.00001
Maximum Time Step: 5
Button "Next"

Output Information (Edit->Flow and Transport Parameters->Output Information)
Print Options:
Check T-Level Information
Keep Evey n time steps: 1
Check Screen Output
Check Press Enter at the End
Print Times: Count: 8
Update
Print Times: 0.05, 0.1, 0.25, 0.5 1, 2, 3, 5
Button "Next"

Water Flow - Iteration Criteria (Edit->Flow and Transport Parameters->Water Flow Parameters->Iteration Criteria)
Leave default values as follows:
Maximum Number of Iterations: 10
Water Content Tolerance: 0.001
Pressure Head Tolerance: 1
Lower Optimal Iteration Range: 3
Upper Optimal Iteration Range: 7
Lower Time Step Multiplication Factor: 1.3
Upper Time Step Multiplication Factor: 0.7
Lower Limit of the Tension Interval: 0.0001
Upper Limit of the Tension Interval: 10000
Initial Condition: In Pressure Heads
Button "Next"

Water Flow - Soil Hydraulic Model (Edit->Flow and Transport Parameters->Water Flow Parameters->Hydraulic Properties Model)
Radio button - van Genuchten-Mualem
Radio button - No hysteresis
Button "Next"

Water Flow - Soil Hydraulic Parameters (Edit->Flow and Transport Parameters->Water Flow Parameters ->Soil Hydraulic Parameters)
Select Silt from Soil Catalog
Button "Next"

Solute Transport – General Info (Edit->Flow and Transport Parameters->Solute Transport Parameters->General Information)

Leave default values except
Number of Solution Concentration Combinations: 2
Button "Next"

Solute Transport – Solute Compositions (Edit->Flow and Transport Parameters->Solute Transport Parameters->Solution Compositions)

Solution Concentrations [meq/L]

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

Adsorption Concentrations [meq/kg]

Ca	Mg	Na	K
0.5	0	9.5	0

Precipitated Concentrations [meq/kg]: all zeros
Button "Next"

Solute Transport - Solute Transport Parameters (Edit->Flow and Transport Parameters->Solute Transport Parameters->Solute Reaction Parameters)

Leave default values except
Bulk Density = 1.4 cm^3/g
Molecular Diffusion, Dw = 2 cm^2/d
Longitudinal Dispersivity, Disp.L = 2 cm
Transverse Dispersivity, Disp.T = 0.2 cm
Cation Exchange Capacity, CEC = 10 meq/kg
Calcium Surface Area = 0 (used only when kinetic precipitation/dissolution is considered)
Dolomite Surface Area = 0 (ditto)
K [Ca/Mg] = 0.896
K [Ca/Na] = 1.158
K [Ca/K] = 0.111
Button "Next"

Solute Transport - Chemical Parameters (Edit->Flow and Transport Parameters->Solute Transport Parameters->Chemical Parameters)

Leave default values
Button "Next"

FE-Mesh - FE-Mesh Parameters (Edit->FE-Mesh->FE-Mesh Parameters)

Horizontal Discretization in X
Count: 45
Update
VerticalHorizontal Discretization in Z
Count: 26
Update

x [cm]	dz [cm]	z [cm]
0	-15	100

3	-15	99
6	-15	97.5
9	-15	95.5
12	-15	93
15	-15	90
16.5	-13.5	87
18	-12	84
19.5	-10.5	81
21	-9	78
22.5	-7.5	75
24	-6	72
25.5	-4.5	69
27	-3	66
28.5	-1.5	62
30	0	58
32	0	54
34	0	50
36.5	0	45
39	0	40
42	0	34
46	0	28
50	0	21
54	0	14
58	0	7
61	0	0
63.5	0	
66	0	
68	0	
70	0	
71.5	-1.5	
73	-3	
74.5	-4.5	
76	-6	
77.5	-7.5	
79	-9	
80.5	-10.5	
82	-12	
83.5	-13.5	
85	-15	
88	-15	
91	-15	
94	-15	
97	-15	
100	-15	

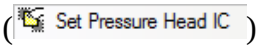
Button "Next"

Default Domain Properties (Edit->Domain Properties->Default Domain Properties)

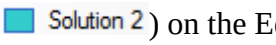
Column h: -200 cm

Column Temp: 25

Column Sol#: 2
Button "Next"

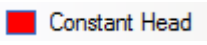
Water Flow Initial Conditions (Edit->Initial Conditions->Pressure Head)
Click on the **Initial Conditions Tab** under the View Window.
Click on the **Pressure Head** on the Navigator Bar.
Select the entire transport domain and then click on *Set Pressure Head IC* (

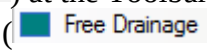
) on the Edit Bar. In the **Water Flow Initial Condition** window, check *Same value for all nodes* and specify *Pressure Head Value* equal to -200 cm.

Solute Transport Initial Conditions (Edit->Initial Conditions->Solution Composition)
Click on the **Solution Composition** on the Navigator Bar.
Select the entire transport domain and then click on *Solution 2* (

) on the Edit Bar.

Water Flow Boundary Conditions (Edit->Boundary Conditions->Water Flow)
Click on the **Boundary Conditions Tab** under the View Window.

a) Click on Zoom by Rectangle () at the Toolbar (or View-> Zoom by Rectangle) and zoom on the left furrow.
   Select *Constant Head* (

) from the Edit Bar, select bottom of the left furrow and 4 nodes on the side, specify 6 cm with *Equilibrium from the lowest located nodal point*.
b) Click on *View All* () at the Toolbar (or View->View All).
   Select *Free Drainage* (

) from the Edit Bar, and select the entire bottom of the transport domain.
c) On the Navigator Bar double click on *Solute Transport*
   Click on Display codes on the Edit Bar (

) and check that "-1" (or "+1") is displayed in the furrow. This means that solution composition 1 will be applied with the irrigation water.
   Uncheck "Display Codes" again.

Observation Nodes
Click on the **Domain Properties Tab** under the View Window.
On the Navigator Bar click on *Domain Properties – Observation Nodes* (or Insert->Domain Properties->Observation Nodes).
Click on the Insert command on the Edit Bar and specify 5 points arbitrarily in the transport domain between the furrow and the bottom of the transport domain.

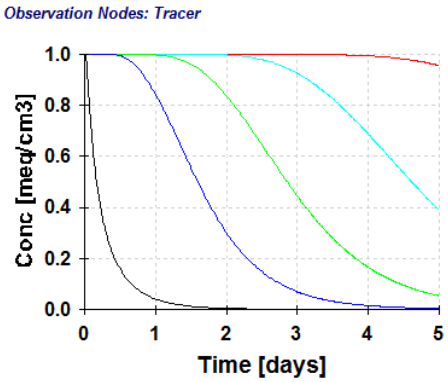
Save
Save the project using the Save command () on the Toolbar (or File->Save).

Run Calculations
Click the Calculate Current Project command () on the Toolbar (or Calculation->Calculate Current Project)

OUTPUT:
Click on the **Results Tab** under the View Window.

Results – Other Information: Observation Points (from the Navigator Bar, or Results->Observation Points from menu)

Pressure Heads
Water Contents
Concentrations



Results – Other Information: Boundary Fluxes (from the Navigator Bar, or Results->Boundary Information->Boundary Fluxes from menu)

Constant Boundary Flux
Free Drainage Boundary Flux

Results – Other Information: Cumulative Fluxes (from the Navigator Bar, or Results->Boundary Information->Cumulative Fluxes from menu)

Constant Boundary Flux
Free Drainage Boundary Flux

Results – Other Information: Solute Fluxes (from the Navigator Bar, or Results->Boundary Information->Solute Fluxes from menu)

Constant Boundary Flux
Seepage Face Boundary Flux

Results – Other Information: Chemical Mass Balance Information (from the Navigator Bar, or Results->Mass Balance Information from menu)

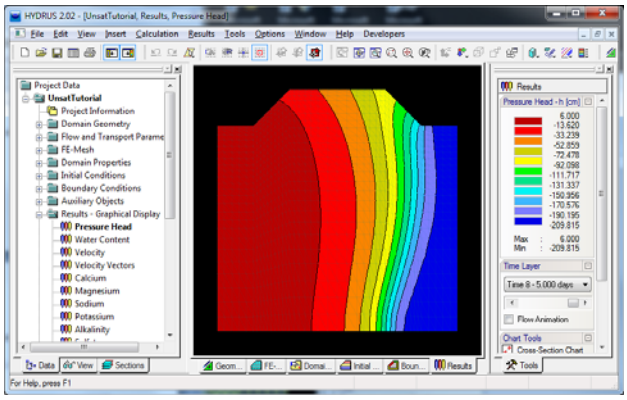
Results – Graphical Display: Pressure Heads (from the Navigator Bar, or Results->Display Quantity->Pressure Heads from menu)

Use Listbox *Time Layer* or *Slidebar* on the Edit Bar to view results for different print times
Check *Flow Animation*
Select different display modes using Options->Graph Type

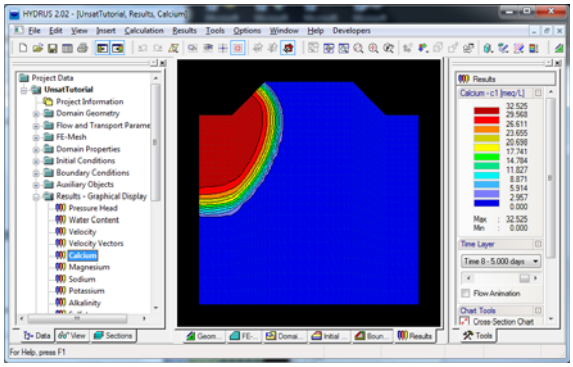
Results – Graphical Display: Water Contents (from the Navigator Bar, or Results->Display Quantity->Water Contents from menu)

Results – Graphical Display: Concentrations (from the Navigator Bar, or Results->Display Quantity->Concentrations from menu)

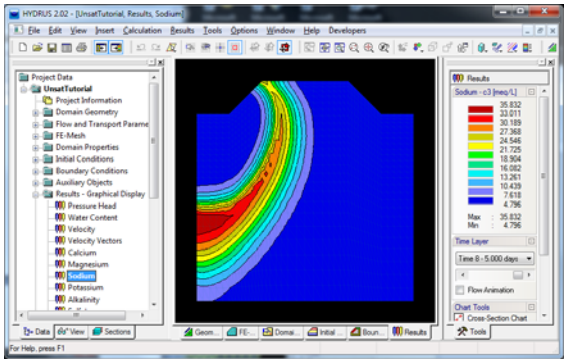
Results – Graphical Display: Velocity Vectors (from the Navigator Bar, or Results->Display Quantity->Velocity Vectors from menu)



Pressure heads (*t*=5 d)



Soluble Calcium (*t*=5 d)



Soluble Sodium (*t*=5 d)

Different Modifications of the Basic Run

1. Considering the effects of the solution composition on the hydraulic conductivity

Project Manager (File->Project Manager)

Select " UnsatchemFurrow"
Button "Copy"
Enter New Name: UnsatchemFurrow 1
Description: Considering the effects of the solution composition on the hydraulic conductivity
Button "OK"
Button "Open" UnsatchemFurrow 1

Solute Transport – Chemical Parameters (Edit->Flow and Transport Parameters->Solute Transport Parameters->Chemical Parameters)

Check "Conductivity Reduction due to Chemistry"
Button "OK"

Re-Run Calculations

Click the *Calculate Current Project* command on the Toolbar (or Calculation→Calculate Current Project)

Results – Graphical Display: Pressure Heads (from the Navigator Bar, or Results->Display Quantity->Pressure Heads from menu)

Use Listbox *Time Layer* or *Slidebar* on the Edit Bar to view results for different print times.

It is clear that the movement of moisture front was dramatically slowed down. Rerun the simulation for longer simulation time.

Time Information (Edit->Flow and Transport Parameters->Time Information)

Final Time: 50 d
Initial Time Step: 0.0001
Minimum Time Step: 0.00001
Maximum Time Step: 5
Button "Next"

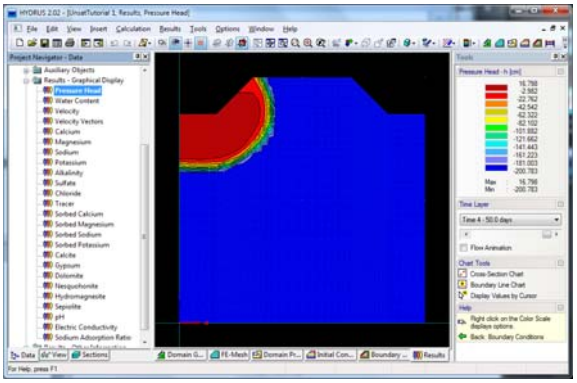
Output Information (Edit->Flow and Transport Parameters->Output Information)

Print Options:
Print Times: Count: 4
Update
Print Times: 5, 10, 25, 50 d
Button "Next"

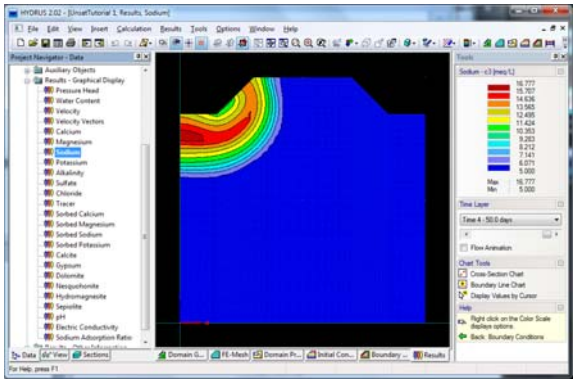
Re-Run Calculations

Click the *Calculate Current Project* command on the Toolbar (or Calculation→Calculate Current Project)

Results – Graphical Display: Pressure Heads and other variables (from the Navigator Bar, or Results->Display Quantity->Pressure Heads from menu)



Pressure heads (*t*=50 d)



Soluble Sodium (*t*=50 d)

Compare results with the previous run

2. Using high quality water for irrigation

Project Manager (File->Project Manager)

Select " UnsatchemFurrow"
Button "Copy"
Enter New Name: UnsatchemFurrow 2
Description: Using high quality water for irrigation
Button "OK"
Button "Open" UnsatchemFurrow 2

Solute Transport – Solute Compositions (Edit->Flow and Transport Parameters->Solute Transport Parameters->Solution Compositions)

Solution Concentrations [meq/L]

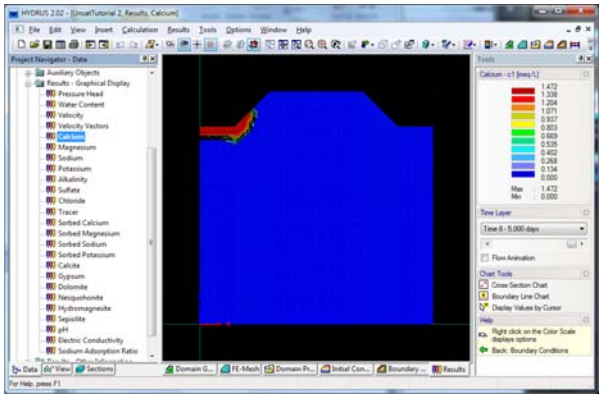
Ca	Mg	Na	K	Alk	SO4	Cl	Tracer
1.5	0.5	2	0	0.5	2.5	1	0
0.2	0	4.8	0	0.4	0	4.6	1

Button "Next"

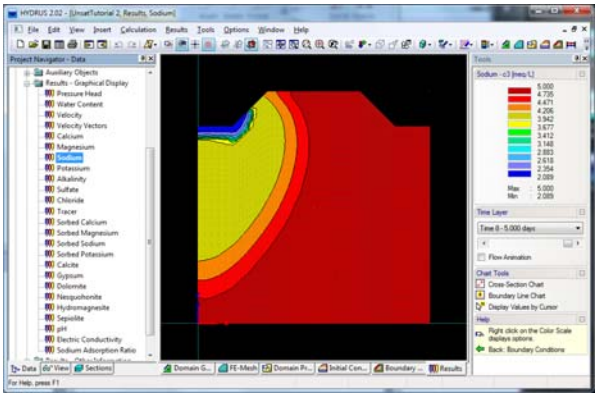
Re-Run Calculations

Click the *Calculate Current Project* command on the Toolbar (or Calculation→Calculate Current Project)

Results – Graphical Display: Pressure Heads and other variables (from the Navigator Bar, or Results->Display Quantity->Pressure Heads from menu)



Soluble Calcium (t=5 d)



Soluble Sodium (t=5 d)

3. Using high quality water for irrigation and assuming presence of calcite in the profile (and either instantaneous or kinetic dissolution).

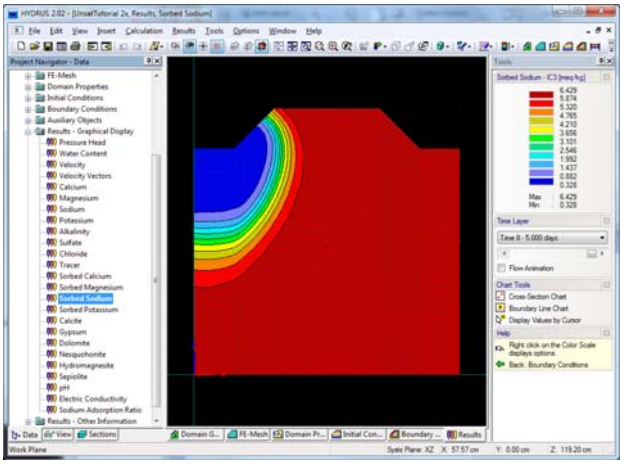
Project Manager (File->Project Manager)

Select " UnsatchemFurrow"
Button "Copy"
Enter New Name: UnsatchemFurrow 2
Description: Using high quality water for irrigation, instantaneous calcite
Button "OK"
Button "Open" UnsatchemFurrow 3a

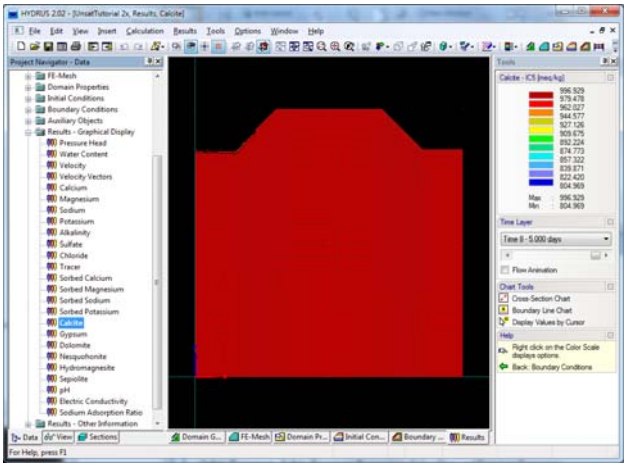
Solute Transport – Solute Compositions (Edit->Flow and Transport Parameters->Solute Transport Parameters->Solution Compositions)

Precipitated Concentrations [meq/kg]:
Calcite = 1000
Button "Next"

Run Calculations



Sorbed Sodium



Calcite

Project Manager (File->Project Manager)

Select " UnsatchemFurrow"
Button "Copy"
Enter New Name: UnsatchemFurrow 3a
Description: Using high quality water for irrigation, kinetic calcite
Button "OK"
Button "Open" UnsatchemFurrow 3b

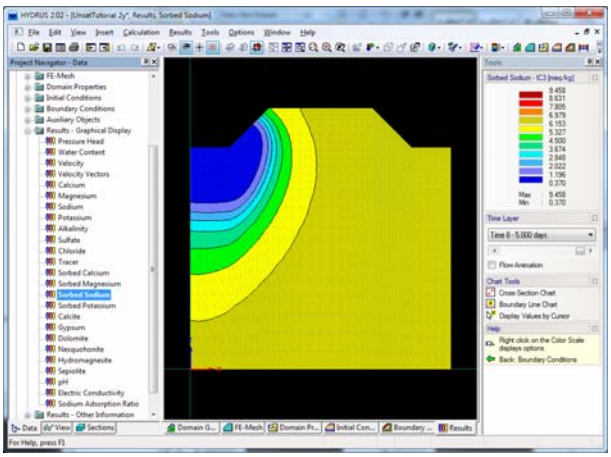
Solute Transport - Solute Transport Parameters (Edit->Flow and Transport Parameters->Solute Transport Parameters->Solute Reaction Parameters)

Leave old values except
Calcium Surface Area = 0.02 [m2/L]
Button "Next"

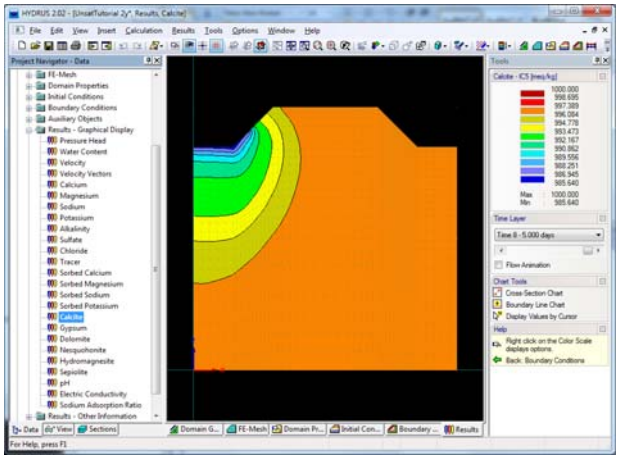
Solute Transport - Chemical Parameters (Edit->Flow and Transport Parameters->Solute Transport Parameters->Chemical Parameters)

Leave default values
Check "Kinetic Precipitation/Dissolution"
Button "Next"

Run Calculations



Sorbed Sodium



Calcite

4. Using different irrigation waters for irrigation

Project Manager (File->Project Manager)

Select " UnsatchemFurrow"
Button "Copy"
Enter New Name: UnsatchemFurrow 4
Description: Using different irrigation waters
Button "OK"
Button "Open" UnsatchemFurrow 4

Time Information (Edit->Flow and Transport Parameters->Time Information)

T-Level Information: Every n Time Steps: 5
Final Time: 5 d
Check "Time-Variable Boundary Conditions" and set the "Number of Time-Variable Boundary Records" equal to 2.
Button "Next"

Output Information (Edit->Flow and Transport Parameters->Output Information)

Print Options:
Print Times: Count: 6
Update
Print Times: 0.5, 1, 2, 3, 4, 5 d
Button "Next"

Solute Transport – General Info (Edit->Flow and Transport Parameters->Solute Transport Parameters->General Information)

Leave default values except
Number of Solution Concentration Combinations: 3
Button "Next"

Solute Transport – Solute Compositions (Edit->Flow and Transport Parameters->Solute Transport Parameters->Solution Compositions)

Solution Concentrations [meq/L]

Ca	Mg	Na	K	Alk	SO4	Cl	Tracer
32.6	0	4.8	0	0.4	32	5	0
0.2	0	4.8	0	0.4	0	4.6	1
2	0	2	0	0.5	2.5	1	**2**

Button "Next"

Variable Boundary Conditions (Edit->Flow and Transport Parameters->Variable Boundary Conditions)

Time	Var.H-1	cValue1
2.5	6	1
5	6	3

Water Flow Boundary Conditions (Edit->Boundary Conditions->Water Flow)
Click on the **Boundary Conditions Tab** under the View Window.

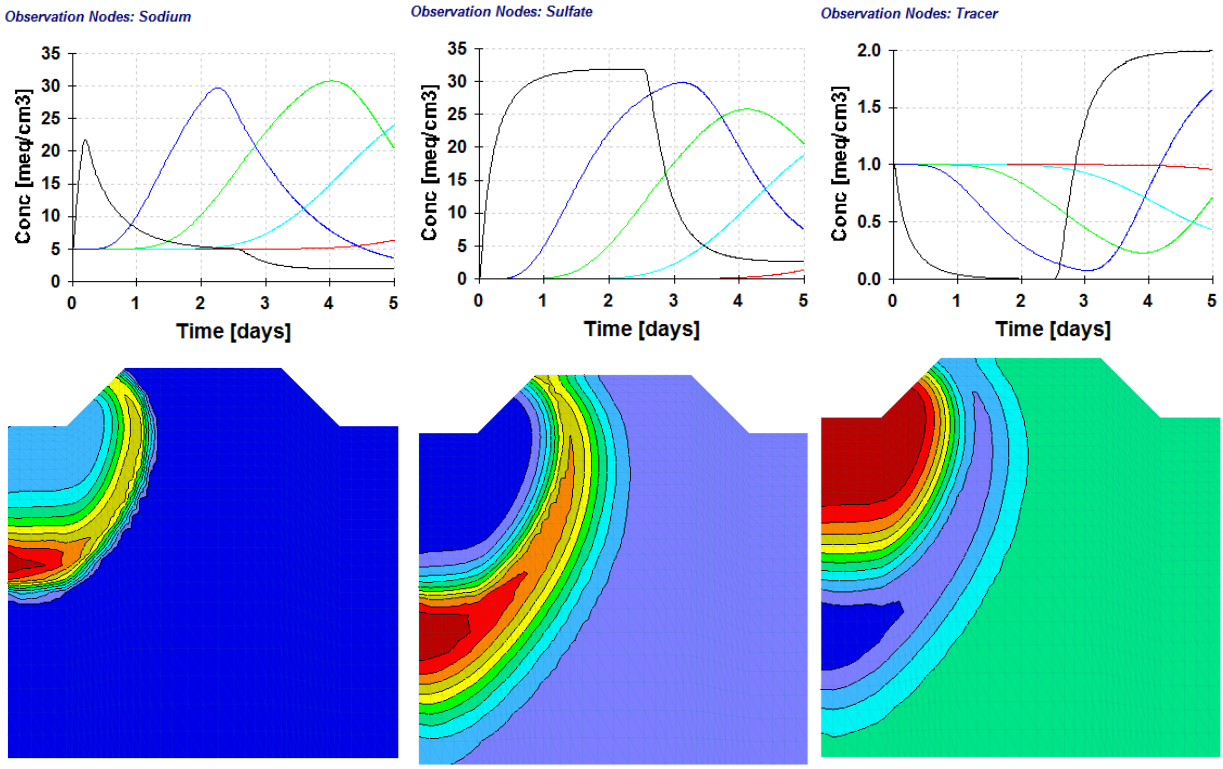
Click on Zoom by Rectangle ( ) at the Toolbar (or View-> Zoom by Rectangle) and zoom on the left furrow.

Select *Variable Head* (Variable Head 1) from the Edit Bar, and overwrite the *Constant Head BC* with *Variable Head BC* (bottom of the left furrow and 4 nodes on the side)

Re-Run Calculations

Click the *Calculate Current Project* command on the Toolbar (or Calculation→Calculate Current Project)

Results – Graphical Display: Pressure Heads and other variables (from the Navigator Bar, or Results->Display Quantity->Pressure Heads from menu)



Calcium Sodium Tracer