

## Example Problem W-1

### Aqueous Flow in Saturated and Unsaturated Porous Media

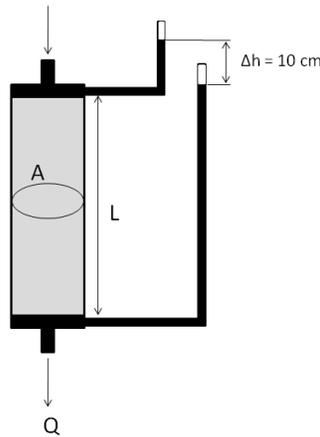
**Abstract:** *The user is introduced to the development of input files for successful simulation of flow problems. The first problem is a simple 1D vertical, single-phase aqueous flow system. Through manipulation of input file parameter values and boundary conditions, various saturated and unsaturated systems are obtained.*

#### Problem Description

Single-phase aqueous flow is simulated with the Water mode (STOMP-W) of the STOMP simulator. As for all modes of the simulator, solute transport can be included. An example of solute transport for STOMP-W is discussed in Problem W-3. This simulation describes flow in a 1-m long column (Figure 1). At the top of the column, a pressure head of 10-cm of water is imposed. The bottom outlet is set to be level with the top of the column. The boundary conditions at the top and bottom result in a pressure difference of 10 cm of water and causes vertical flow in a downward direction. The rate of flow in this column is given by Darcy's Law:

$$Q = AK \frac{\Delta h}{L} \quad (1)$$

where  $Q$  is the flow rate ( $\text{m}^2/\text{s}$ ),  $A$  is the cross-sectional area perpendicular to flow direction ( $\text{m}^2$ ),  $K$  is the hydraulic conductivity ( $\text{m/s}$ ),  $L$  is the length of the column ( $\text{m}$ ),  $h$  is the hydraulic head ( $\text{m}$ ) and  $\Delta$  denotes the change in  $h$  over the length  $L$ .



**Figure 1.** Vertical 1D flow in a column of cross-sectional area  $A$  and length  $L$ .

The hydraulic head at a specific point,  $h$  is the sum of the pressure head and the elevation,

$$h = p / \rho g + z \quad (2)$$

where  $p$  is the water pressure (Pa),  $\rho$  is the water density ( $\text{kg}/\text{m}^3$ ),  $g$  is the acceleration of gravity ( $\text{m}/\text{s}^2$ ), and  $z$  is the elevation (m).

The saturated hydraulic conductivity is defined as

$$K = \frac{k\rho g}{\mu} \quad (3)$$

where  $k$  is the intrinsic permeability ( $\text{m}^2$ ) and  $\mu$  is the dynamic viscosity (Pa s).

The standard information regarding the simulation is stated in the *Simulation Title Card*. Among other information, it contains the name of the authors and a short description of the problem.

```
#-----  
~Simulation Title Card  
#-----  
v3.1,  
STOMP Example Problem W-1,  
Mart Oostrom/Mark White,  
PNNL,  
June 03,  
15:00,  
1,  
Vertical flow in 1D column,
```

The *Solution Control Card* specifies that the execution mode option is Normal and that the Water mode (STOMP-W) is used. There is one execution time period that starts at  $t=0$  seconds and lasts for one day. The initial time step is 1 sec. and the maximum time step 1 day. The time step acceleration factor is 1.25, the maximum number of Newton-Raphson iterations is 8, and the convergence criterion is  $1.e-6$ . A total of 10000 time steps are allowed and all interfacial averaging occurs according to the defaults listed in Table 4.3 (page 4.10) in the User's Guide (White and Oostrom, 2006) and in the online User's Guide on the [Initial Conditions Description](#) page.

```
#-----  
~Solution Control Card  
#-----  
Normal,  
STOMP-W,  
1,  
0,s,1,d,0.001,s,1,d,1.25,8,1.e-6,  
10000,  
0,
```

The domain is divided into 10 uniform cells in the z-direction. The dimensions of each cell are 0.1x0.1x0.1 m.

```
#-----  
~Grid Card  
#-----  
Uniform Cartesian,  
1,1,10,  
0.1,m,  
0.1,m,  
0.1,m,
```

A porous medium named 'sand' is assigned to all cells.

```
#-----
~Rock/Soil Zonation Card
#-----
1,
Sand,1,1,1,1,1,10,
```

The sand is assigned a particle density of 2650 kg/m<sup>3</sup> and both the total porosity and diffusive porosity are 0.4. The specific storage is not specified, and is therefore calculated based on the default compressibility and specified porosity. The Millington and Quirk tortuosity model is specified.

```
#-----
~Mechanical Properties Card
#-----
Sand,2650,kg/m^3,0.4,0.4,,Millington and Quirk,
```

The hydraulic conductivity in the z-direction is 10.0 m/day. Conductivities in the other two directions are not needed.

```
#-----
~Hydraulic Properties Card
#-----
Sand,,,,10.0,hc m/day,
```

The air-water retention relations have to be provided in the *Saturation Function Card*. If the domain remains saturated during a run, the specified values are not used. The capillary pressure-saturation relation is described using the van Genuchten formulation (van Genuchten 1980):

$$\bar{s}_l = \left[ 1 + \left( \beta_{gl} \alpha h_{gl} \right)^n \right]^{-m}; \quad \bar{s}_l = \frac{s_l - s_{lr}}{1 - s_{lr}}; \quad m = 1 - \frac{1}{n} \quad (4)$$

where  $\beta_{gl}$  is the gas-aqueous scaling factor,  $h_{gl}$  is the gas-aqueous capillary head (m) and  $s_l$  is the liquid saturation. The sand has a van Genuchten  $\alpha$  parameter of 2.5 1/m, a van Genuchten  $n$  parameter of 2.0, and an irreducible water saturation  $S_{lr}$  of 0.10.

```
#-----
~Saturation Function Card
#-----
Sand, Van Genuchten, 2.5, 1/m, 2.0, 0.10,
```

The *Aqueous Relative Permeability Card* is required for all modes. For this simulation, the Mualem pore-size distribution model is used. The Mualem porosity distribution function (van Genuchten 1980) is defined as:

$$k_{rl} = \sqrt{s_l} \left\{ 1 - \left( 1 - s_l^{(1/m)} \right)^m \right\}^2 \quad (5)$$

The van Genuchten  $m$  value is computed according  $m = 1 - 1/n$ .

```
#-----
~Aqueous Relative Permeability Card
#-----
Sand, Mualem,
```

It is assumed that the column is initially completely saturated with a hydrostatic pressure gradient of -9793.52 Pa/m. This gradient is the product of the liquid density and gravitational acceleration. It is further assumed that the aqueous pressure at the top of the column is atmospheric at 101325 Pa. Given the distance from the top to the lowest node is 0.95 m, the aqueous pressure at the lowest node is computed as  $101325 + 0.95 * 9793.52 = 110629$  Pa.

```
#-----
~Initial Conditions Card
#-----
Gas Pressure, Aqueous Pressure,
1,
Aqueous Pressure, 110629, Pa, -9793.52, 1/m, 1, 1, 1, 1, 10,
```

The pressure is described at both boundaries using a Dirichlet boundary condition. The aqueous pressure at the top is equivalent to a head of 10 cm of water. The prescribed value at the bottom boundary indicates an outlet water level located at the top boundary. This value is computed as  $101325 + 1.0 * 9793.52 = 111119$  Pa.

```
#-----  
~Boundary Conditions Card  
#-----  
2,  
top,dirichlet,  
1,1,1,1,10,10,1,  
0,d,102304,Pa,  
bottom,dirichlet,  
1,1,1,1,1,1,1,  
0,d,111119,Pa,
```

The *Output Options Card* indicates that reference node variables will be written to the screen and the *output* file for all nodes in the problem after completion of every time step. The default output time units are in hr and the output length units in cm. The screen, output file, and plot file significant digits are all 6. The reference node variables are aqueous saturation, aqueous pressure, aqueous hydraulic head and the node-centered volumetric aqueous flux in the vertical direction. The reference node variables are written to the *output* file. Besides the final *plot* file, there is one additional *plot* file being generated at  $t = 12$  hr. A total of 5 plot file variables are specified. The first one is included to avoid the writing of restart files at the prescribed plot file times. The rest of the plot file variables are identical to the reference node variables.

```
#-----  
~Output Options Card  
#-----  
10,  
1,1,10,  
1,1,9,  
1,1,8,  
1,1,7,  
1,1,6,  
1,1,5,  
1,1,4,  
1,1,3,  
1,1,2,  
1,1,1,  
1,1,hr,cm,6,6,6,  
4,  
aqueous saturation,,  
aqueous pressure,Pa,  
aqueous hydraulic head,cm,  
znc aqueous volumetric flux,cm/day,  
1,  
12,hr,  
5,  
no restart,,
```

aqueous saturation,,  
aqueous pressure,Pa,  
aqueous hydraulic head,cm,  
znc aqueous volumetric flux,cm/day,

A total of 2 fluxes and associated integral amounts will be written to a file called *surface*.

```
#-----  
~Surface Flux Card  
#-----  
2,  
Aqueous Volumetric Flux,l/day,l,top,1,1,1,10,10,  
Aqueous Volumetric Flux,l/day,l,bottom,1,1,1,1,1,
```

### References

van Genuchten, MT. 1980. "A Closed-Form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils," *Soil Science Society of America Journal*, 44:892-898.

White, MD, Appriou, D, Bacon, DH, Fang, Y, Freedman, V, Rockhold, ML, Ruprecht, C, Tartakovsky, G, White, SK, Zhang, F. 2015. *STOMP Online User Guide*. Pacific Northwest National Laboratory: Richland Washington. [stomp-userguide.pnnl.gov](http://stomp-userguide.pnnl.gov).

White, MD and M Oostrom. 2006. *Stomp Subsurface Transport over Multiple Phases, Version 4.0, User's Guide*, PNNL-15782.

### Exercises

1. Run the base STOMP-W problem by executing an appropriate executable. Look at the output on the screen for all individual nodes. Verify that one output file, two plot files and one surface file are created. View the contents of each file.
2. Decrease the porosity in the *Mechanical Properties Card* to 0.2. Execute the run and view the results. Change variable back to old value.
3. Reduce the hydraulic conductivity by a factor 10. Run the simulation and view the results. Change variable back to old value.
4. Increase the pressure at the top of domain to represent a 20-cm water head. Execute the run and view the results. Change variable back to old value.
5. Add a second porous medium named 'silt' to the input file. The silt should occupy the lower 50 cm of the flow cell. The upper half of the column should still be sand. Give the silt the same properties as the sand, except for a 1 m/day hydraulic conductivity.

Change the simulation end time to 10 days. Additions are needed to the *Rock/Soil Zonation, Mechanical Properties, Hydraulic Properties, Saturation Function, Aqueous Relative Permeability, and Solution Control Cards*. Execute the simulation and view the results.

6. Reduce the hydraulic conductivity of the silt to 0.1 m/day. Run the simulation and view the results. Change variable back to 1 m/day.
7. Change the number of Rock/Soil Types to 1 and allow the sand to occupy the complete column. Leave all the silt-related lines in the input file because they are needed later. However, they will not be read when the number of Rock/Soil Types is set to 1. Change the *Boundary Conditions Card* to the following:

```
1,  
bottom,dirichlet,  
1,1,1,1,1,1,3,  
0,d,111119,Pa,  
1,d,102304,Pa,  
10,d,102304,Pa,
```

Comment on the changes in this card. Predict the effect of the imposed change. Run the simulation and view the results.

8. Change the van Genuchten  $\alpha$  parameter to 1.25 1/m. Run the simulation and view the results. Change the variable back to the original value.
9. Change the van Genuchten  $n$  parameter to 4.0. Run the simulation and view the results. Change the variable back to the original value.
10. Change the van Genuchten saturation function of the sand to Brooks and Corey as follows:

```
Sand,Brooks and Corey,0.4,m,1.0,0.10,,
```

Run the simulation and view the results. Change the line back to the original line containing the van Genuchten saturation function.

11. Increase the Rock/Soil Types back to 2 to include the silt. Change the van Genuchten  $\alpha$  parameter of the silt to 1.25 1/m. Run the simulation and view the results. Change the variable back to the original value.

## Input File

```
#-----  
~Simulation Title Card  
#-----  
v3.1,  
STOMP Example Problem W-1,  
Mart Oostrom/Mark White,  
PNNL,  
June 03,  
15:00,  
1,  
Vertical flow in 1D column,  
  
#-----  
~Solution Control Card  
#-----  
Normal,  
STOMP-W,  
1,  
0,s,1,d,0.001,s,1,d,1.25,8,1.e-6,  
10000,  
0,  
  
#-----  
~Grid Card  
#-----  
Uniform Cartesian,  
1,1,10,  
0.1,m,  
0.1,m,  
0.1,m,  
  
#-----  
~Rock/Soil Zonation Card  
#-----  
1,  
Sand,1,1,1,1,1,10,  
  
#-----  
~Mechanical Properties Card  
#-----  
Sand,2650,kg/m^3,0.4,0.4,,Millington and Quirk,  
  
#-----  
~Hydraulic Properties Card  
#-----  
Sand,,,,,10.0,hc m/day,  
  
#-----  
~Saturation Function Card  
#-----  
Sand,Van Genuchten,2.5,1/m,2.0,0.10,,
```

```
#-----  
~Aqueous Relative Permeability Card  
#-----  
Sand,Mualem,,  
  
#-----  
~Initial Conditions Card  
#-----  
Gas Pressure, Aqueous Pressure,  
1,  
Aqueous Pressure,110629,Pa,,,,,-9793.52,1/m,1,1,1,1,1,10,  
  
#-----  
~Boundary Conditions Card  
#-----  
2,  
top,dirichlet,  
1,1,1,1,10,10,1,  
0,d,102304,Pa,  
bottom,dirichlet,  
1,1,1,1,1,1,1,  
0,d,111119,Pa,  
  
#-----  
~Output Options Card  
#-----  
10,  
1,1,10,  
1,1,9,  
1,1,8,  
1,1,7,  
1,1,6,  
1,1,5,  
1,1,4,  
1,1,3,  
1,1,2,  
1,1,1,  
1,1,hr,cm,6,6,6,  
4,  
aqueous saturation,,  
aqueous pressure,Pa,  
aqueous hydraulic head,cm,  
znc aqueous volumetric flux,cm/day,  
1,  
12,hr,  
5,  
no restart,,  
aqueous saturation,,  
aqueous pressure,Pa,  
aqueous hydraulic head,cm,  
znc aqueous volumetric flux,cm/day,
```

```
#-----
~Surface Card
#-----
2,
Aqueous Volumetric Flux,l/day,l,top,1,1,1,10,10,
Aqueous Volumetric Flux,l/day,l,bottom,1,1,1,1,1,
```

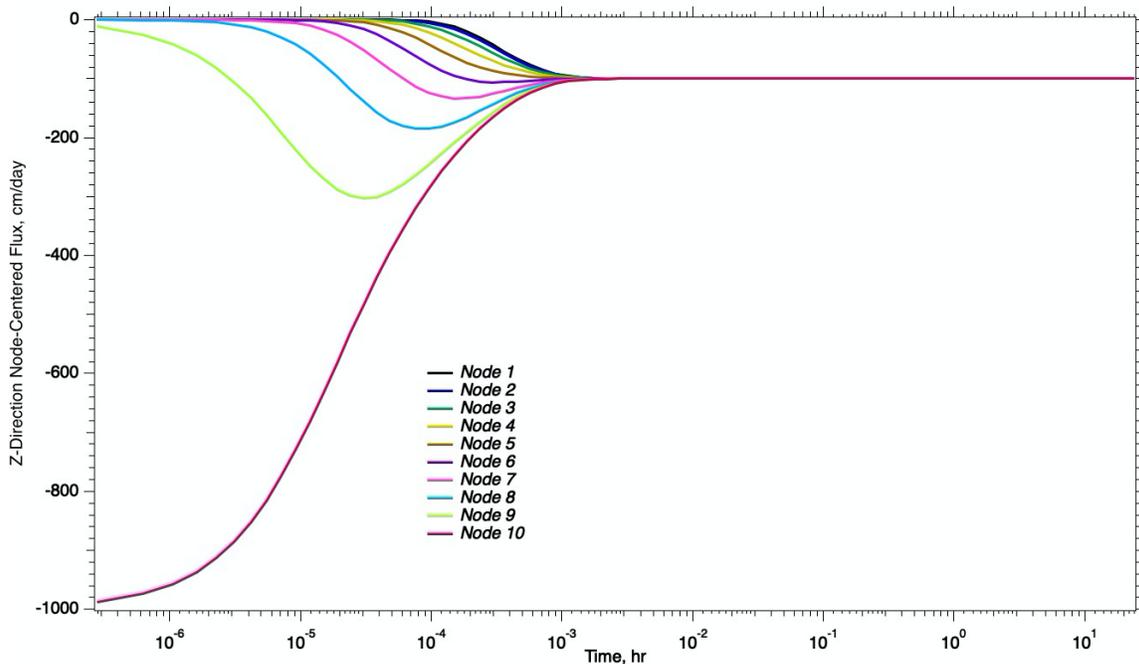
## Solutions to Selected Exercises

### Exercise 1

Initially the pressure distribution in the column is hydrostatic, resulting in no flow conditions. Suddenly 10 cm of water is imposed above the cylinder, creating a hydraulic gradient and in resulting downward flow. The system reacts quickly to the boundary condition and the steady state flow of  $q = -100 \text{ cm/day}$  is reached rapidly.

### Exercise 2

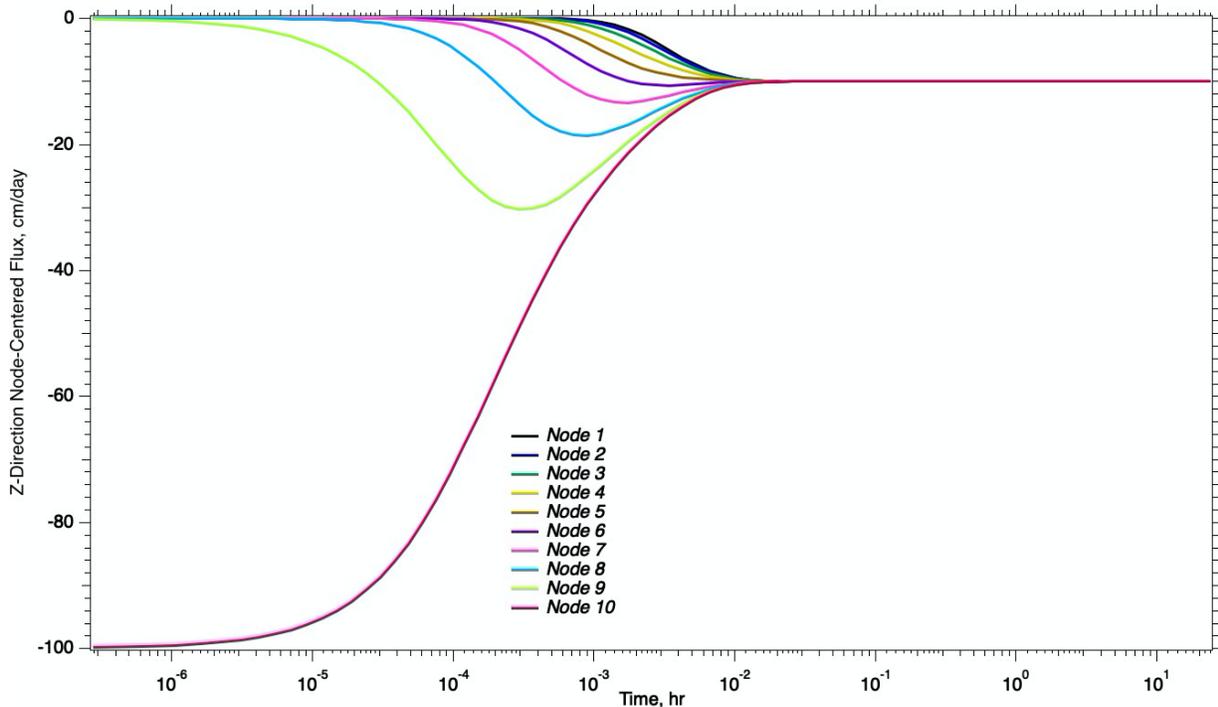
The simulator allows changes in porous media porosity independent of other hydrologic properties. For an aqueous saturated system at moderate pressures, the Darcy velocity is independent of porosity; therefore, the transient and steady-state flow field is identical to that shown in Figure 2.



**Figure 2.** Flow in a saturated porous media column in response to a suddenly imposed 10-cm head (Darcy Velocity transients).

### Exercise 3

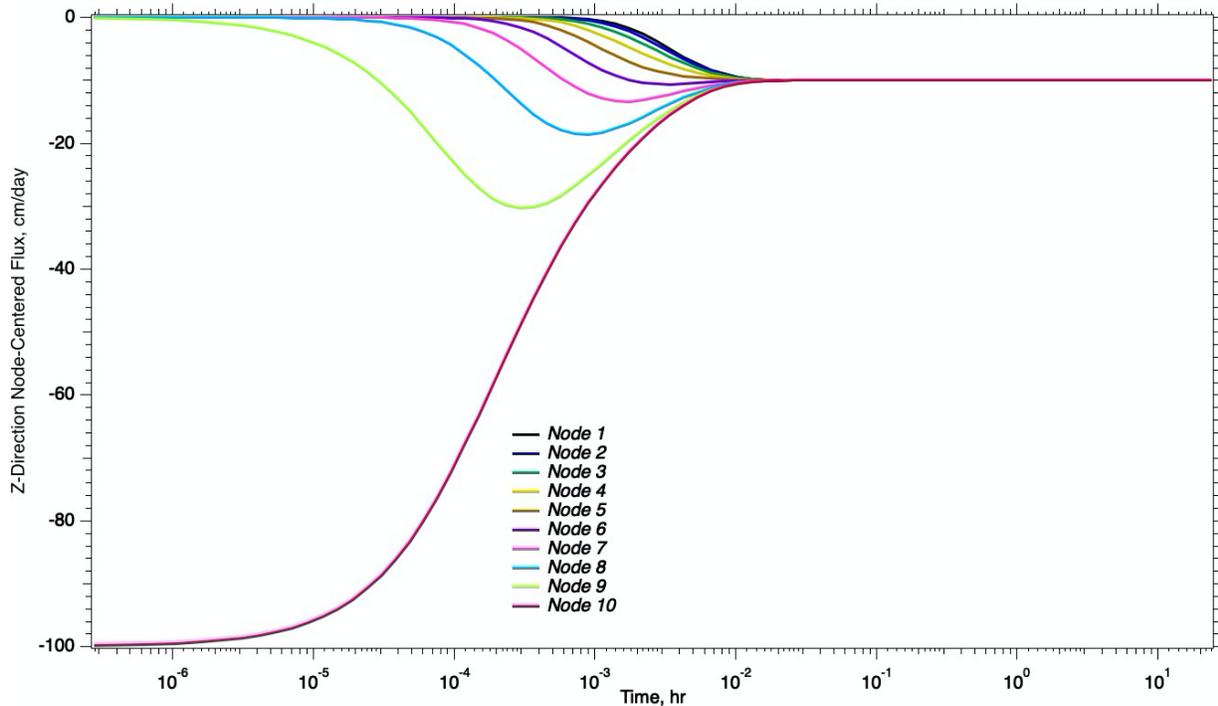
Darcy's Law implies that the flow rate is proportional to the hydraulic conductivity. Reducing the hydraulic conductivity by a factor of 10 reduces the flow rate and the time required to reach steady-flow conditions by a factor of 10, as seen by comparing Figures 2 and 3. The steady state flow rate is  $q = -10$  cm/day.



**Figure 3.** Flow in a saturated porous media column in response to a suddenly imposed 10-cm head (Hydraulic conductivity = 1 m/day, Darcy velocity transients).

### Exercise 4

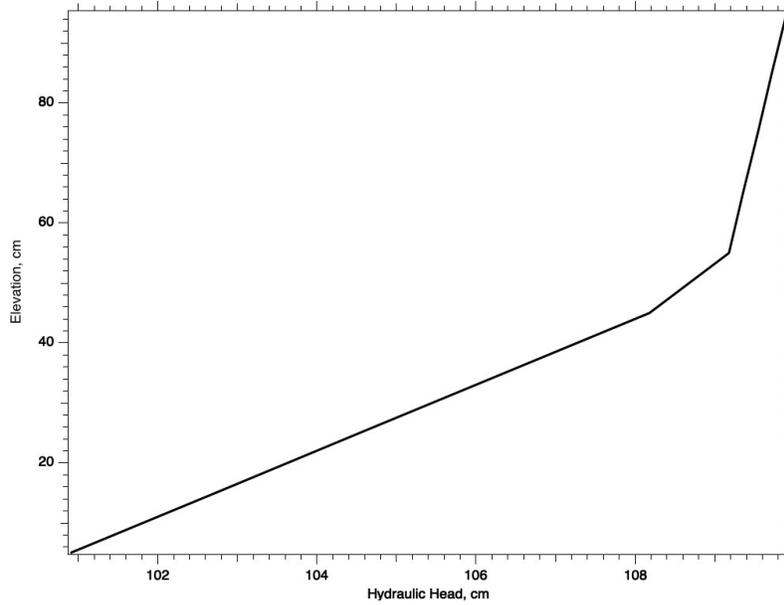
A 20-cm water head is imposed by increasing the boundary pressure on the column top from 102304 to 103283 Pa. Darcy's Law states that flow rate is proportional to the hydraulic gradient. Doubling the hydraulic gradient doubles the flow rate to  $q = -200$  cm/day, but does not alter the time required to reach steady-flow conditions, as shown in Figure 4.



**Figure 4.** Flow in a saturated porous media column in response to a suddenly imposed 20-cm head (Ponded head = 20 cm, Darcy velocity transients).

### Exercise 5

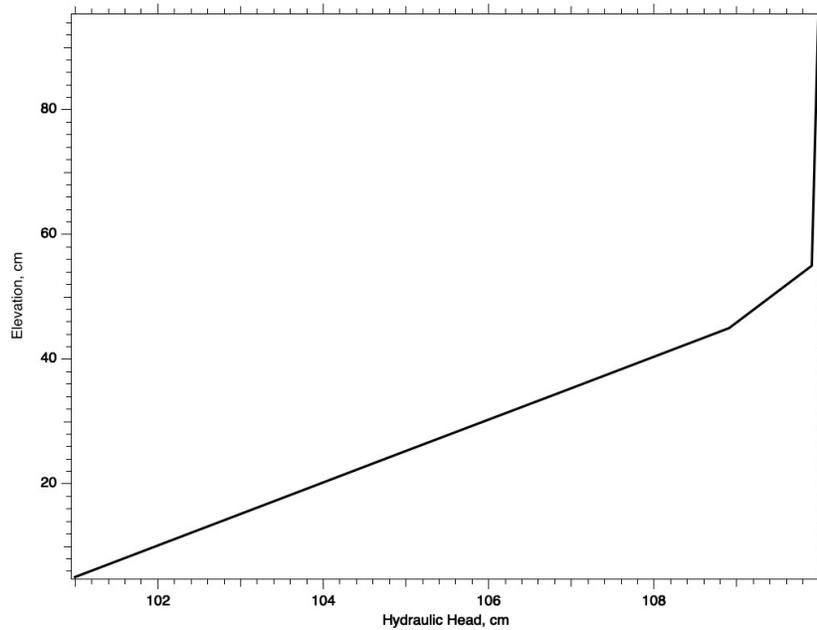
The addition of the silt decreases the overall hydraulic conductivity of the system and reduces the steady state flow rate to -18.19 cm/day. Continuity requires that the flow rate is the same throughout the sand and the silt. The hydraulic head in each soil is linearly distributed, but there is a slope discontinuity at the soils interface. The pressure gradient in the silt is greater than in the sand, as seen in Figure 5.



**Figure 5.** Flow in a saturated porous media column in response to a suddenly imposed 10-cm head (Silt hydraulic conductivity = 1.0 m/day, Hydraulic head at 10 days).

### Exercise 6

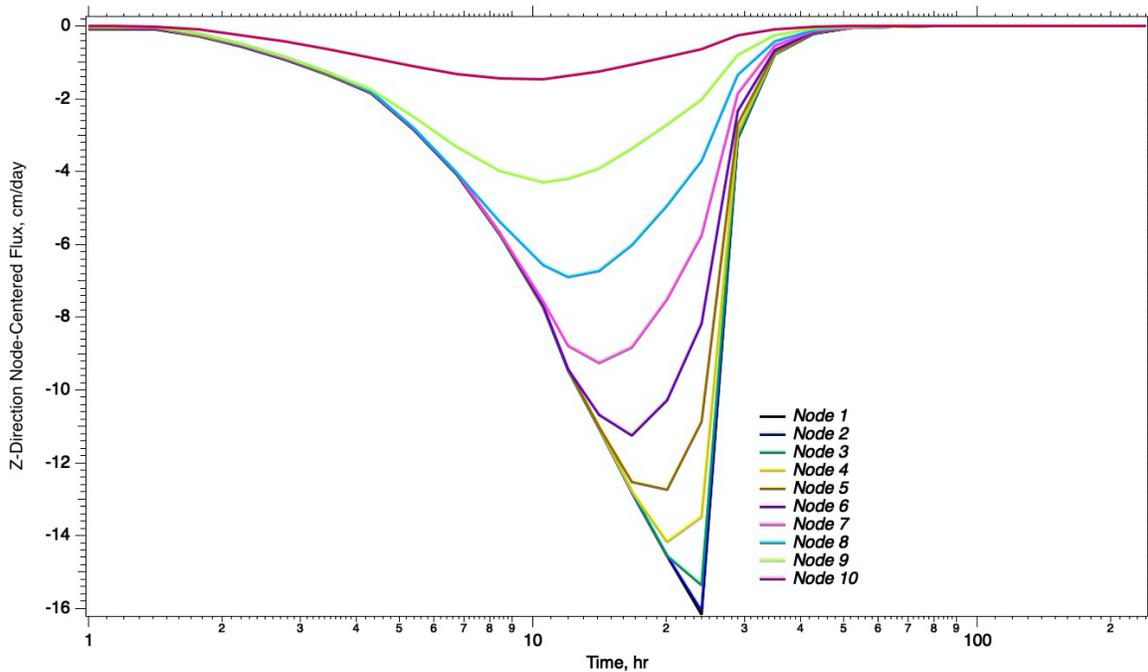
Reducing the hydraulic conductivity of the silt to 0.1 m/day reduces the flow rate to -1.98 cm/day. The 10.0 cm of head is mostly being used to force the fluid through the silt.



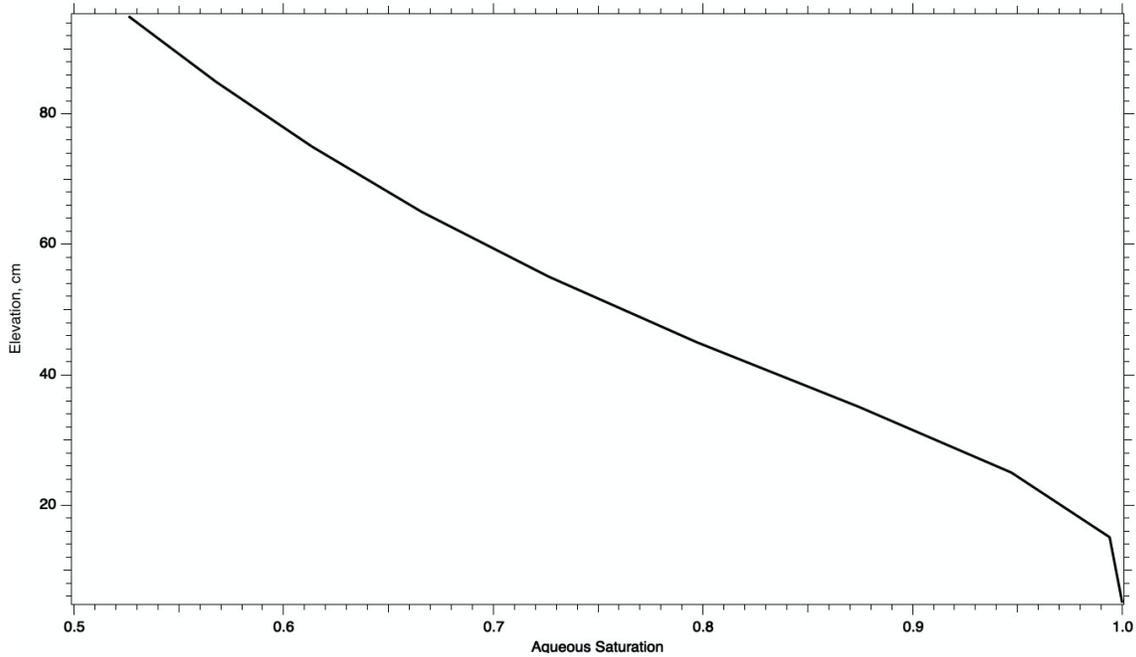
**Figure 6.** Flow in a saturated porous media column in response to a suddenly imposed 10-cm head (Silt hydraulic conductivity = 0.1 m/day, Hydraulic head at 10 days).

### Exercise 7

For this exercise the upper pressure boundary condition is removed, eliminating the ponded water. The lower boundary condition is converted to transient form, representing a falling pressure over the first day, followed by a constant pressure boundary for 9 days. These boundary conditions model controlled drainage of a saturated soil column; where, the pressure head on the column bottom drops 90 cm over 1 day, followed by a constant head condition for 9 days. Initially water drains quickly from the soil column, until desaturation slows the drainage rate. The drainage rate as indicated by the Darcy velocity at each grid cell is shown in Figure 7. Column drainage becomes minimal after 60 hours. The final drained-column saturation profile is shown in Figure 8.



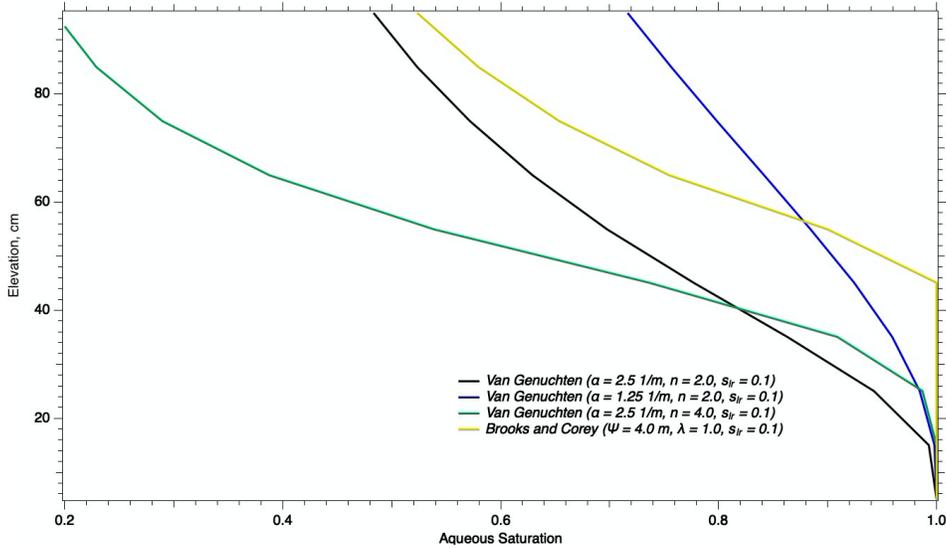
**Figure 7.** Flow in a saturated porous media column in response to a suddenly imposed 10-cm head (Column drainage, Darcy velocity transients).



**Figure 8.** Flow in a saturated porous media column in response to a suddenly imposed 10-cm head (Column drainage, aqueous saturation at 10 days).

### Exercises 8, 9 & 10

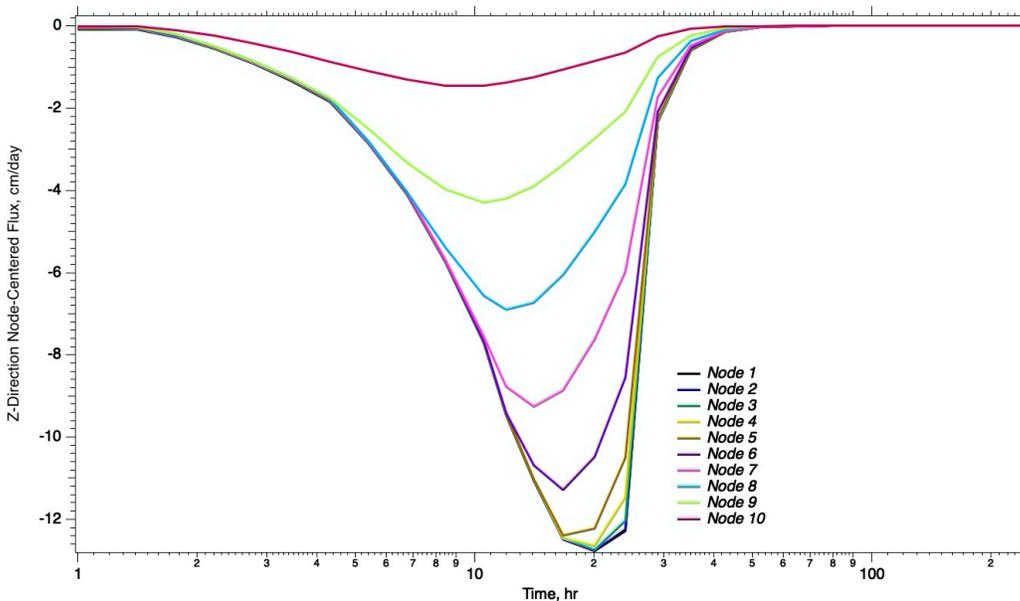
This series of drainage simulations demonstrate differences in saturation profiles for variations in the soil-moisture retention characteristics. Because the simulations are carried to steady-state or near steady-state conditions, while the resulting saturation profiles are different for different saturation function parameters and models as shown in Figure 9, they are insensitive to the relative permeability function.



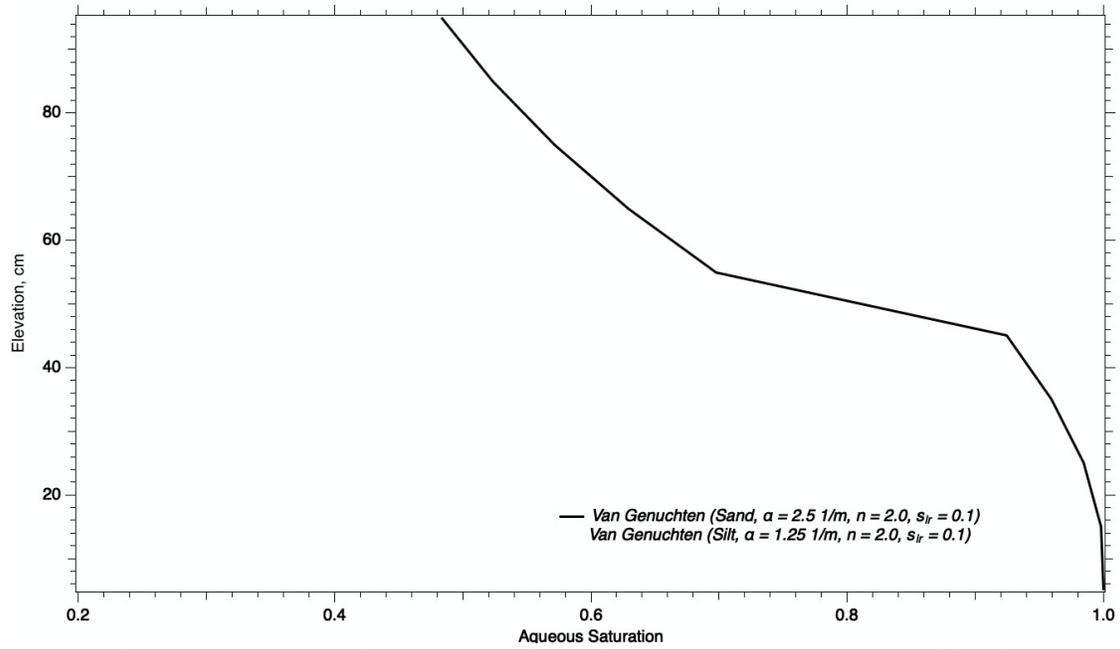
**Figure 9.** Flow in a saturated porous media column in response to a suddenly imposed 10-cm head (Saturation function variants, aqueous saturation at 10 days).

**Exercise 11**

The lower hydraulic conductivity of the silt prevents the drainage from completing in the 10-day period, as shown in Figure 10. Although drainage was incomplete, the split-soil system yields a composite drainage curve, as shown in Figure 11.



**Figure 10.** Flow in a saturated porous media column in response to a suddenly imposed 10-cm head (Silt layer, Darcy velocity transients).



**Figure 11.** Flow in a saturated porous media column in response to a suddenly imposed 10-cm Head (Silt layer, aqueous saturation at 10 days).