Faculty Environmnetal Sciences

Hydrodynamics in porous media

Seminar notes

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2017

Contents

Chapter 1

Introduction

1.1 Expectations

This document is a collection of tutorials with the Dual Richards Unsaturated Equation Solver (DRUtES). The tutorials are in 1D for simplicity. We start with simple flow models such as heat conduction through a wall, followed by simple infiltration, then we move on to coupled models with examples covering coupled heat and water flow, and finally coupled water flow and contaminant transport.

1.2 Software

1. Install *DRUtES*. You can get *DRUtES* from the github repository drutes-dev or download it from the drutes.org website.

2. Follow website instructions on drutes.org for the installation.

3. Working R installation (optional, to generate plots you can execute freely distributed R script)

4. The branch *tutorial* will work with all tutorials.

Chapter 2

Heat module

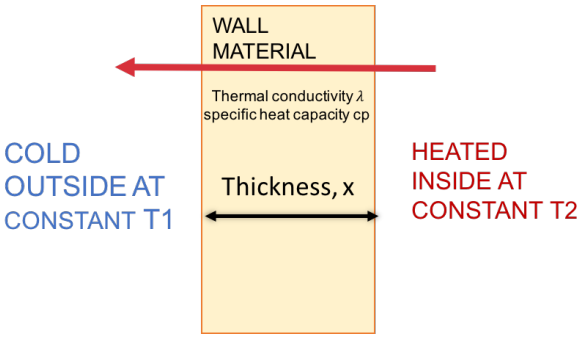
2.1 Heat module - Part 1

2.1.1 Goal and Complexity

Complexity: Beginner

Prerequisites: None

The goal of this tutorial is to get familiar with the *DRUtES* heat module and *DRUtES* configuration in 1D by simulating heat conduction through a 20 cm thick wall.



Heat flow is important in the soil. To simplify, we're assuming heat flow through a wall. We test different insulation materials by assigning different heat capacities and thermal conductivity values of several real-world materials.

In this tutorial three configuration files will be modified step by step. All configuration files are located in the folder *drutes.conf* and respective subfolders.

1. For selection of the module, dimension and time information we require *global.conf*. *global.conf* is located in *drutes.conf / global.conf*.

2. To define the mesh or spatial discretization in 1D, we require *drumesh1D.conf*. *drumesh1D.conf* is located in *drutes.conf / mesh / drumesh1D.conf*.

3. To define heat conduction, we require *heat.conf*. *heat.conf* is located in *drutes.conf / heat / heat.conf*.

DRUtES works with configuration input file with the file extension .conf. Blank lines and lines starting with # are ignored. The input mentioned in this tutorial therefore needs to be placed one line below the mentioned keyword, unless stated otherwise.

We use the heat equation for one-dimensional problems given as

$$C\frac{\partial T}{\partial t} = \kappa_T \frac{\partial^2 T}{\partial x^2}, \tag{2.1}$$

where C is the volumetric heat capacity [J.K^{-1}], T is the temperature [K], and κ_T is the thermal conductivity [W.m^{-1}.K^{-1}].

2.1.2 Scenarios

For all scenarios, we assume that the wall is between a heated room, which is maintaining a constant temperature of 20 °C, and the outside world during winter, which for the sake of simplicity is at a constant temperature of 0 °C. The outside temperature and the heated room temperature are our boundary conditions. They define the limits of our spatial domain. They give us a lot of information on our problem. We already know the solution of our problem at the boundaries and they do not change over time. This type of boundary condition is called **Dirichlet boundary condition**. We assume 1D flow. This means that we are only interested in one-direction. Although this might seem drastic, it only means that the other directions are homogeneous and do not provide us with more information.

We can assume a simple domain set-up as in Fig. 2.1. What is missing is the material properties defining the heat conduction. These can be found in Tab. 2.1 for three different materials: stone concrete, sand stone and cotton.

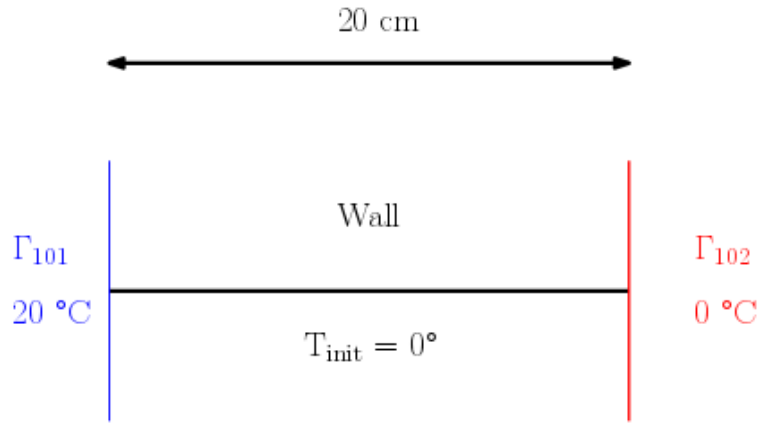


Figure 2.1: Domain set-up for 1D heat conduction through a wall with two constant Dirichlet conditions.

Scenario 1

Heat conduction through a 20 cm thick stone concrete wall.

global.conf: Choose correct model, dimension, time discretization and observation times.

1. Open ***global.conf*** in a text editor of your choice.

2. Model type: Your first input is the module. Input is **heat**.

Table 2.1: Material properties needed for scenarios.

Material	specific heat capacity C_p [J kg^{-1} K^{-1}]	density ρ [kg m^{-3}]	thermal conductivity κ_T [W m^{-1} K^{-1}]
Stone concrete	750	1400	1.7
Sand stone	920	2800	1.7
Cotton	1340	1550	0.04

3. Initial mesh configuration

   (a) The dimension of our problem is 1. Input: 1.

   (b) We use the internal mesh generator. Input: 1.

4. Error criterion (not needed here, leave at default value)

   (a) Maximum number of iteration of the Picard method: 20

   (b) h tolerance: 1e-2.

5. Time information

   (a) Time units are in hours: input h

   (b) Initial time: 1e-3.

   (c) End time: 24.

   (d) Minimum time step: 1e-6.

   (e) Maximum time step: 0.1.

6. Observation time settings

   (a) Observation time method: 2

   (b) Set file format of observation: pure. Output in 1D is always in raw data. Different options will not impact output in 1D.

   (c) Make sequence of observation time: n

(d) Number of observation times: 11

(e) Observation time values: 2, 4, 6, 8, 10, 12 ,14, 16, 18, 20, 22. Use a new line for each input. *DRUtES* automatically generates output for the initial time and final time. DRUtES will generate 13 output files, e.g. *heat_ temperature-x.dat*, where x is the number of the file and not the output time. The initial time is assigned an x value of 0.

7. Observation point settings

   (a) Observation point coordinates: 0.0, 0.2. Use a new line for each input. *DRUtES* will generate 2 output files, e.g. *obspt_ heat-x.out*, where x is the ID of the observation point.

8. Ignore other settings for now.

9. **Save** *global.conf*!!!

*drumesh*1*D.conf*: Mesh definition, i.e. number of materials and spatial discretization

1. Open ***drumesh1D.conf*** in a text editor of your choice.

2. Geometry information: 0.2 m - domain length

3. Amount of intervals: 1

4.

density	bottom	top
0.005	0	0.2

5. number of materials: 1

6.

id	bottom	top
1	0	0.2

heat.conf: Heat module after Sophocleous (1979).

1. Open *heat.conf* in a text editor of your choice.

2. Couple with Richards equation: n

3. Number of materials or layers: 1

4. Specific heat capacity of the wall material:
   750 J kg^{-1} K^{-1} x 1400 kg m^{-3} = 1.05E6 J m^{-3} K^{-1} = $\frac{1.05E6 \text{ W s m}^{-3} \text{ K}^{-1}}{3600 \text{ s h}^{-1}}$
   = 291 W h m^{-3} K^{-1}.

5. Specific heat capacity of liquid: 0

6. Anisotropy: There is no anisotropy. The value is 0.

7. Heat conductivity of the wall material: 1.7 W m^{-1} K^{-1}.

8. There is NO heat convection of water: 0.

9. The initial temperature is 0°C across the entire domain: 0.

10. There is no heat source: 0.

11. We have 2 boundaries at both ends of the wall. We assume a constant temperature of 0 °C outside. We assume the inside is heated and the temperature maintained at exactly 20°C. We therefore know the temperature at the boundaries. We also know that these values do not change in time. They can be describes as time-constant Dirichlet boundary conditions.

boundary id	boundary type	use bc.dat	value
101	1	n	20.0
102	1	n	0.0

12. Save heat.conf.

Run scenario 1

Run the simulation in the terminal console.

1. Make sure you are in the right directory.

2. To execute *DRUtES*:
   $ bin/drutes

3. After the simulation finishes, to generate png plots execute provided R script:
   $ Rscript drutes.conf/heat/heatplots.R concrete

4. The output of the simulation can be found in the folder out

Tasks for scenario 1

1. How long does it take for the temperature distribution to become linear between the two observation points?

2. How large is the steady state heat flux through the wall?

3. Let's assume a wall area of A=15 m^2. Use the observation point at the boundary between the wall and the inside of room. How large was the cumulated heat loss after 24 h. How much will be lost after 48 h when the set-up does not change?

Result of scenario 1

Question 1

Figure 2.2 shows that the temperature distribution becomes linear quite quickly and reaches a steady state after observation time 2, which was set to 4 h. Figure 2.3 shows the heat flux ϕ_p in observation points 1 (red) and 2 (blue) bordering the wall to the outside and heated inside, respectively. The heat flux is extremely large at observation point 2 in the beginning. Observation point 2 evidently defines the boundary between the wall and the heated inside. After approximately 3 hours, the heat flux of observation point 1 and 2 become identical. This occurs when the simulation reaches steady state and a linear temperature distribution. Figure 2.3 allows a more exact estimation of when the system becomes steady state.

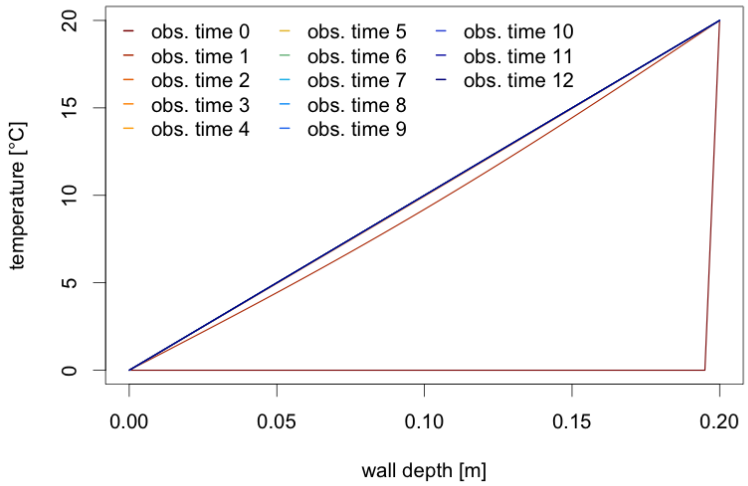


Figure 2.2: Plot of observation times for stone concrete generated with Rscript heatplots.R

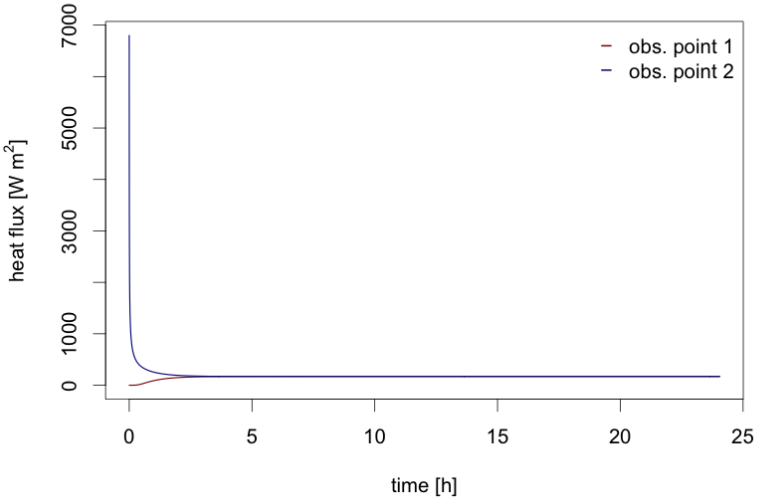


Figure 2.3: Heat flux at observation points 1 and 2 for stone concrete generated with Rscript heatplots.R

Question 2

The constant heat flux value is at ϕ_p=170 W m^{-2}. This value can also be calculated using the equation:

$$\phi_{\mathrm{p}} = -\kappa_T \frac{dT}{dx} = -1.7 \frac{20-0}{0.2} = 170 \text{ W m}^{-2}$$

Question 3

Figure 2.4 shows the cumulative heat flux in observation points 1 and 2, both ends of the wall. The cumulative heat flux after 24 h at observation point is 4468 W m^{-2}. With a wall area of 15 m^2 this results in $Q = 4468$ W h $m^{-2} \cdot$ 15 $m^2 = 67020$ W h. For the next 24 h, the heat flux will be constant at 170 W m^{-2}. The total heat loss will therefore be $Q = 170$ W $m^{-2} \cdot 24$ h $\cdot$ 15 $m^2 = 61200$ W h.

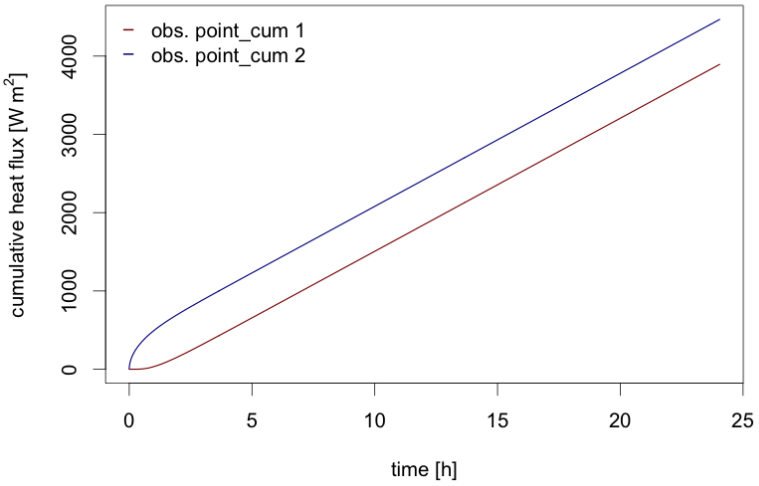


Figure 2.4: Cumulated heat flux at observation points 1 and 2 for stone concrete generated with Rscript heatplots.R

Scenario 2

Heat conduction through a 20 cm thick sandstone wall.

1. Open *heat.conf* in a text editor of your choice.
2. Leave all settings the same, except for specific heat capacity.
3. Replace the specific heat capacity with values of sand stone.
4. Save heat.conf.

Run scenario 2

Run the simulation in the terminal console.

1. Make sure you are in the right directory.
2. To execute *DRUtES*:
   $ bin/drutes
3. After the simulation finishes, to generate png plots execute provided R script:
   $ Rscript drutes.conf/heat/heatplots.R sandstone
4. The output of the simulation can be found in the folder out

Tasks for scenario 2

1. Answer the same questions as for scenario 1. What is different?

Result of scenario 2

Question 1

Figure 2.5 shows that it takes longer for the temperature distribution to become linear in sandstone than in concrete sand. Also taking Fig. 2.6 into account, it takes approximately 5 h. This is because sandstone has a larger specific heat capacity than stone concrete.

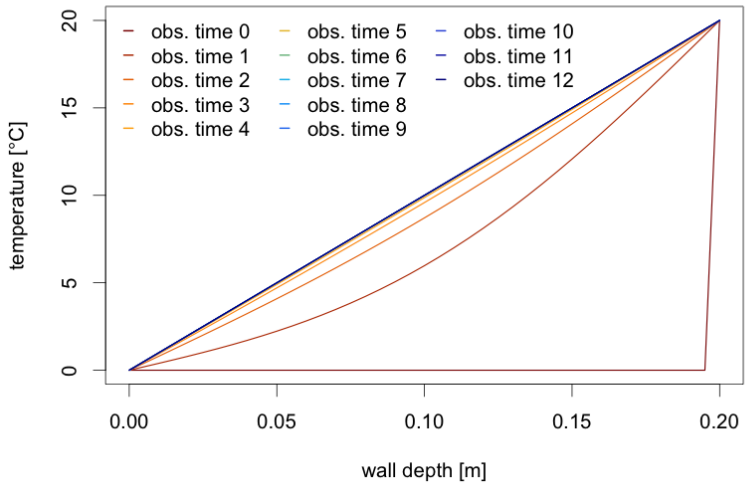


Figure 2.5: Plot of observation times for sandstone generated with Rscript heatplots.R

Question 2

The constant heat flux when the system is in steady state is also at ϕ_p=170 W m^{-2}. Both materials have the same thermal conductivity and therefore the same thermal heat flux.

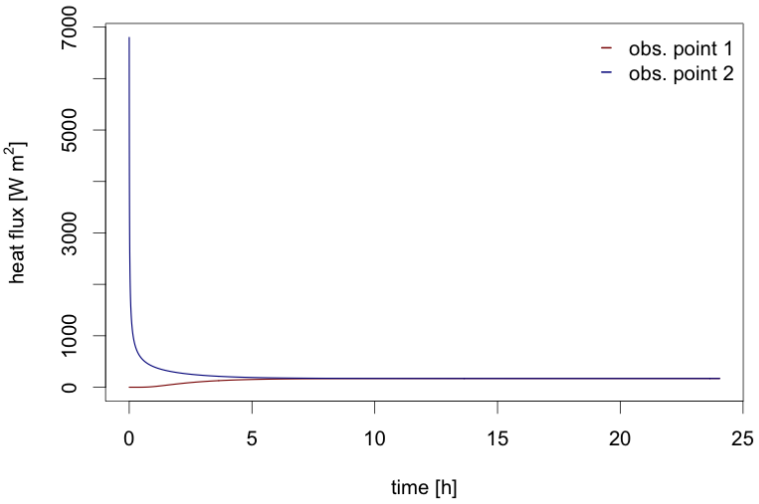


Figure 2.6: Heat flux at observation points 1 and 2 for sandstone generated with Rscript heatplots.R

Question 3

Heat conduction through a 20 cm thick cotton fibre wall.

The cumulative heat flux after 24 h at observation point 2 in sandstone is higher than in concrete stone, namely 5014 W m^{-2}. With a wall area of 15 m^2 this results in Q = 5014 W h $m^{-2} \cdot$ 15 m^2 = 75210 W h. For the next 24 h, the heat flux will be constant at 170 W m^{-2}. The total heat loss will therefore also be Q = 170 W m^{-2} $\cdot$ 24 h $\cdot$ 15 m^2 = 61200 W h.

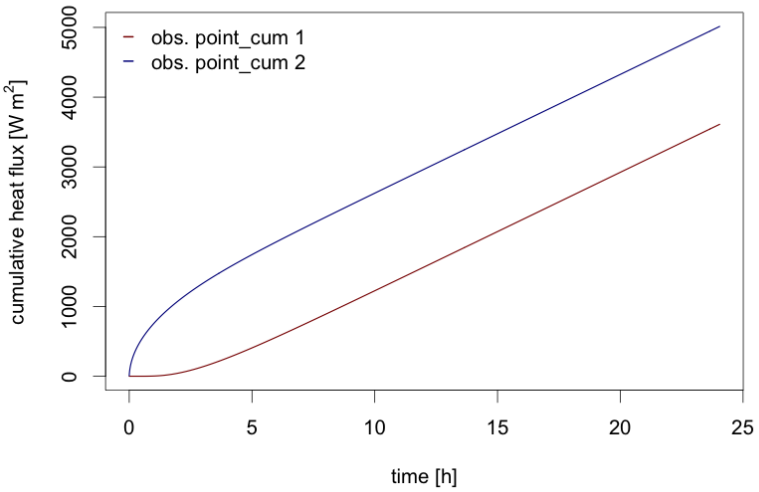


Figure 2.7: Cumulated heat flux at observation points 1 and 2 for sandstone generated with Rscript heatplots.R

Scenario 3

1. Open *heat.conf* in a text editor of your choice.
2. Change the specific heat capacity and thermal conductivity with values of cotton.
3. Save heat.conf.

Run scenario 3

Run the simulation in the terminal console.

1. Make sure you are in the right directory.
2. To execute *DRUtES*:
   $ bin/drutes
3. After the simulation finishes, to generate png plots execute provided R script:
   $ Rscript drutes.conf/heat/heatplots.R cotton
4. The output of the simulation can be found in the folder out

Tasks for scenario 3

1. Answer the same questions as for scenario 1. What is different to scenario 1 and 2?

Result of scenario 3

Question 1

In contrary to scenario 1 and 2, figure 2.8 and 2.9 show that we have not reached steady-state within 24 h. This is because of the very low thermal heat conductivity of cotton fibre.

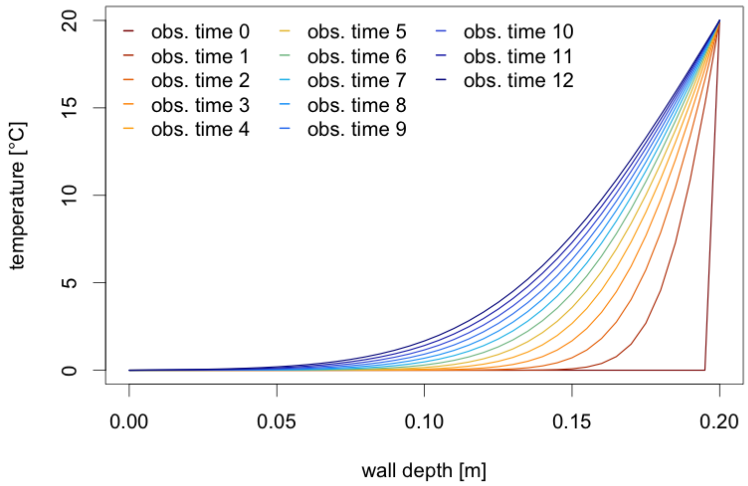


Figure 2.8: Plot of observation times for cotton generated with Rscript heatplots.R

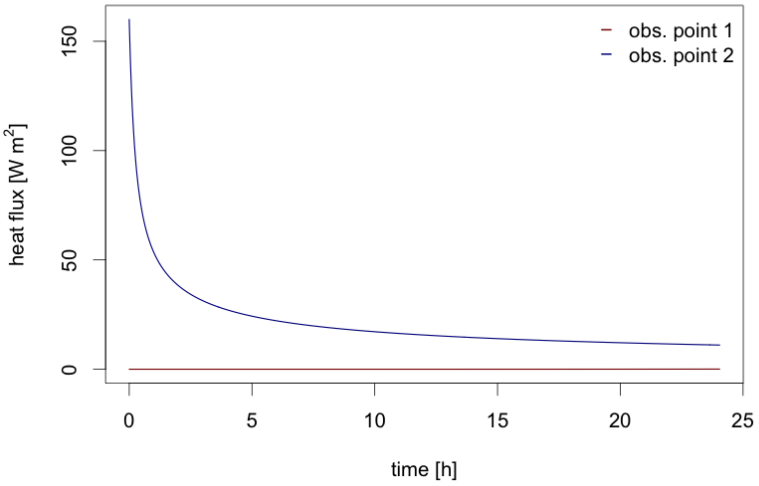


Figure 2.9: Heat flux at observation points 1 and 2 for cotton generated with Rscript heatplots.R

Question 2

We cannot estimate the constant heat flux during steady-state with our results. Using the heat flux equation mentioned during scenario 1, we can calculate the heat flux during steady state:

$$\phi_{\mathrm{p}} = -\kappa_T \frac{dT}{dx} = -0.04 \frac{20 - 0}{0.2} = 4 \text{ W m}^{-2}$$

Question 3

The cumulative heat flux after 24 h at observation point 2 in sandstone is higher than in concrete stone, namely 503 W m^{-2}, so about a tenth of sandstone and stone concrete. With a wall area of 15 m^2 this results in $Q = 503$ W h $m^{-2} \cdot$ 15 $m^2 = 7545$ W h.

Since the system is not in steady state, it is difficult to estimate the heat loss for the next 24 h. The answer has to be evaluated numerically by increasing the end time to 48 h.

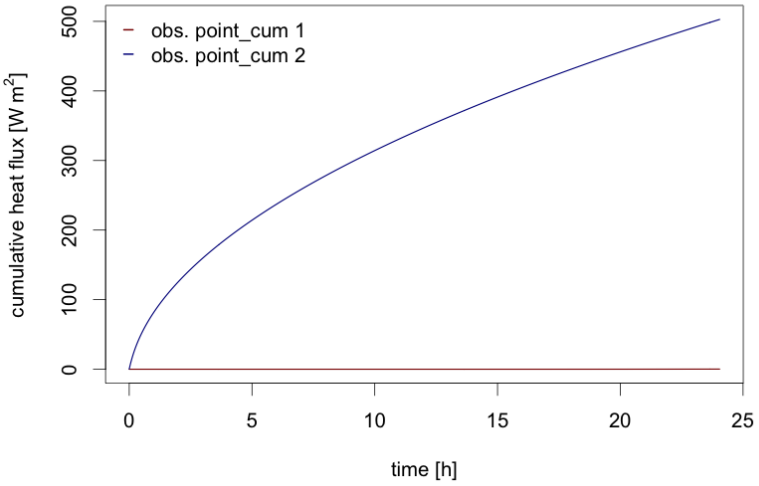


Figure 2.10: Cumulated heat flux at observation points 1 and 2 for sandstone generated with Rscript heatplots.R

2.1.3 Outcome

1. You got familiar with the *DRUtES* heat module in 1D.
2. You simulated heat conduction through a wall with different materials
3. You understand the effects of different heat capacities and thermal conductivities.
4. You understand the terms *Dirichlet boundary condition*, *initial condition* and *steady state*.

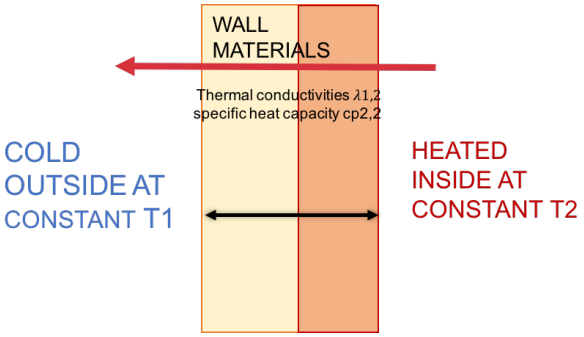
2.2 Heat module - Part 2

2.2.1 Goal and Complexity

Complexity: Beginner

Prerequisites: Tutorial: heat module - part 2.

The goal of this tutorial is to show further applicability of the *DRUtES* heat module in 1D. We simulate heat conduction in a wall with two materials to understand the effects of layering of materials with different thermal properties.



Similar to tutorial 1, three configuration files will be modified step by step. All configuration files are located in the folder *drutes.conf* and respective subfolders.

1. For selection of the module, dimension and time information we require *global.conf*. *global.conf* is located in *drutes.conf* / *global.conf*.

2. To define the mesh or spatial discretization in 1D, we require *drumesh1D.conf*. *drumesh1D.conf* is located in *drutes.conf / mesh / drumesh1D.conf*.

3. To define heat conduction, we require *heat.conf*. *heat.conf* is located in *drutes.conf / heat / heat.conf*.

DRUtES works with configuration input file with the file extension .conf. Blank lines and lines starting with # are ignored. The input mentioned in this tutorial therefore needs to be placed one line below the mentioned keyword, unless stated otherwise.

2.2.2 Scenarios

For all scenarios, we assume that the wall is between a heated room, which is maintaining a constant temperature of 20 °C, and the outside world during winter, which for the sake of simplicity is at a constant temperature of 0 °C.

Table 2.2: Material properties needed for scenarios.

	specific heat capacity	density	thermal conductivity
	c_p	ρ	λ
Material	[J kg^{-1} K^{-1}]	[kg m^{-3}]	[W m^{-1} K^{-1}]
Stone concrete	750	1400	1.7
Cotton	1340	1550	0.04

Scenario 1

Heat conduction through a 20 cm wall. 15 cm are made of stone concrete and 5 cm are made of cotton fibre.

global.conf: Choose correct model, dimension, time discretization and observation times. This is the same as in heat tutorial 1.

1. Open ***global.conf*** in a text editor of your choice.
2. Model type: Your first input is the module. Input is **heat**.
3. Initial mesh configuration
   (a) The dimension of our problem is 1. Input: 1.
   (b) We use the internal mesh generator. Input: 1.
4. Error criterion (not needed here, leave at default value)
   (a) Maximum number of iteration of the Picard method: 20
   (b) h tolerance: 1e-2.

5. Time information
   (a) Time units are in hours: input h
   (b) Initial time: 1e-3.
   (c) End time: 24.
   (d) Minimum time step: 1e-6.
   (e) Maximum time step: 0.1.
6. Observation time settings
   (a) Observation time method: 2
   (b) Set file format of observation: pure. Output in 1D is always in raw data. Different options will not impact output in 1D.
   (c) Make sequence of observation time: n
   (d) Number of observation times: 11
   (e) Observation time values: 2, 4, 6, 8, 10, 12 ,14 ,16, 18, 20, 22. Use a new line for each input. *DRUtES* automatically generates output for the initial time and final time. DRUtES will generate 13 output files, e.g. *heat_ temperature-x.dat*, where x is the number of the file and not the output time. The initial time is assigned an x value of 0.
7. Observation point settings
   (a) Observation point coordinates: 0.0, 0.2. Use a new line for each input. *DRUtES* will generate 2 output files, e.g. *obspt_ heat-x.out*, where x is the ID of the observation point.
8. Ignore other settings for now.
9. Save *global.conf*

*drumesh*1*D.conf*: Mesh definition, i.e. number of materials and spatial discretization. Here is were the configuration files are different to heat tutorial one.

1. Open ***drumesh1D.conf*** in a text editor of your choice.

2. Geometry information: 0.2 m - domain length

3. Amount of intervals: 1

4.

density	bottom	top
0.005	0	0.2

5. Number of materials: 2

6.

id	bottom	top
1	0	0.15
2	0.15	0.2

heat.conf: Heat module after Sophocleous (1979). Here, it is important to make sure everything is defined for 2 layers. 2 lines of input are required, even when the input is identical.

1. Open *heat.conf* in a text editor of your choice.

2. Couple with Richards equation: n

3. Number of materials or layers: 2

4. Specific heat capacity of the wall material: Material 1 is stone concrete:
   750 J kg^{-1} K^{-1} x 1400 kg m^{-3} = 1.05E6 J m^{-3} K^{-1} = $\frac{1.05E6 \text{ W s } m^{-3} \text{ } K^{-1}}{3600 \text{ s } h^{-1}}$
   = 291 W h m^{-3} K^{-1}.
   Material 2 is cotton fibre:
   1340 J kg^{-1} K^{-1} x 1550 kg m^{-3} = 2.08E6 J m^{-3} K^{-1} = $\frac{2.08E6 \text{ W s } m^{-3} \text{ } K^{-1}}{3600 \text{ s } h^{-1}}$
   = 576 W h m^{-3} K^{-1}.

5. Specific heat capacity of liquid: 0 (for both materials)

6. Anisotropy: There is no anisotropy. The value is 0 (for both materials)

7. Heat conductivity of the wall material:
   Material 1: 1.7 W m^{-1} K^{-1}
   Material 2: 0.04 W m^{-1} K^{-1}

8. There is NO heat convection of water: 0 (for both materials)

9. The initial temperature is 0°C across the entire domain: 0 (for both materials)

10. There is no heat source: 0 (for both materials)

11. This is identical to heat tutorial 1. We have 2 boundaries at both ends of the wall. We assume a constant temperature of 0°C outside. We assume the inside is heated and the temperature maintained at exactly 20°C. We therefore know the temperature at the boundaries. We also know that these values do not change in time. They can be describes as time-constant Dirichlet boundary conditions.

boundary id	boundary type	use bc.dat	value
101	1	n	20.0
102	1	n	0.0

12. Save heat.conf.

Run scenario 1

Run the simulation in the terminal console.

1. Make sure you are in the right directory.

2. To execute *DRUtES*:
   $ bin/drutes

3. After the simulation finishes, to generate png plots execute provided R script:
   $ Rscript drutes.conf/heat/heatplots.R concretecotton1

4. The output of the simulation can be found in the folder out

Tasks for scenario 1

1. Describe the temperature distribution. How long does it take for the temperature distribution to become linear between the two observation points?

2. How large is the steady state heat flux through the wall?

3. Let's assume a wall area of A=15 m^2. Use the observation point at the boundary between the wall and the inside of room. How large was the cumulated heat loss 24 h. How much will be lost after 48 h when the set-up does not change?

Result of scenario 1

Question 1

Figure 2.11 shows two distinct linear temperature distributions. The temperature distributions appears to have not changed significantly over the last observation times indicating a steady state. A 5 cm thick cotton fibre wall is between the concrete stone and the heated inside. The overall heat flux at the inside border is therefore quite low as the input of heat has to travel through badly conducting material first.

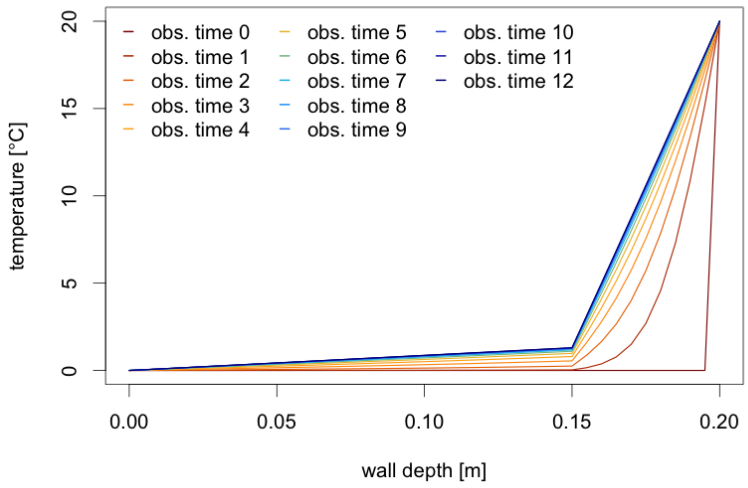


Figure 2.11: Plot of observation times for a wall with a 15 cm outer stone concrete layer and an inner 5 cm cotton fibre layer generated with Rscript heatplots.R

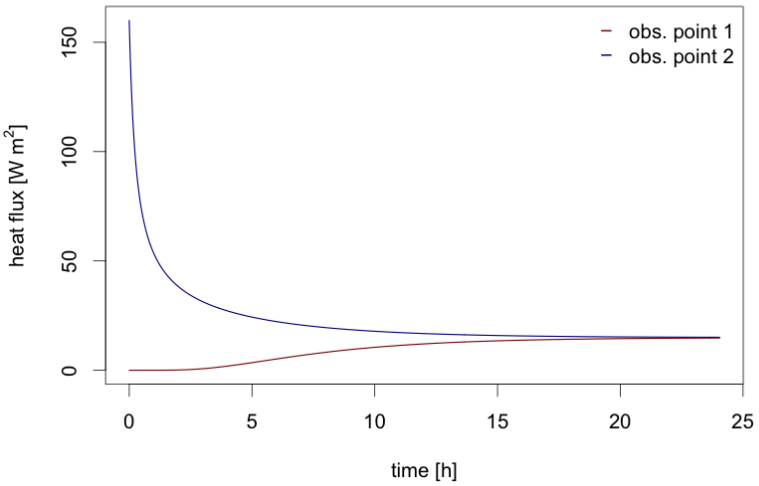


Figure 2.12: Heat flux at observation points 1 and 2 for a wall with a 15 cm outer stone concrete layer and an inner 5 cm cotton fibre layer generated with Rscript heatplots.R

Question 2

Looking at the raw data, it appears that steady-state has not actually been reached, but that the change in heat flux is becoming slower and is converging towards 15 W m^{-2}.

Question 3

Figure 2.13 shows the cumulative heat flux in observation points 1 and 2, both ends of the wall. The cumulative heat flux after 24 h at observation point is 538 W m^{-2}. With a wall area of 15 m^2 this results in $Q = 538$ W h $m^{-2} \cdot$ 15 $m^2 = 8070$ W h. For the next 24 h, the heat flux will be constant at 15 W m^{-2}. The total heat loss will therefore be $Q = 15$ W $m^{-2} \cdot 24$ h $\cdot$ 15 $m^2 = 5400$ W h.

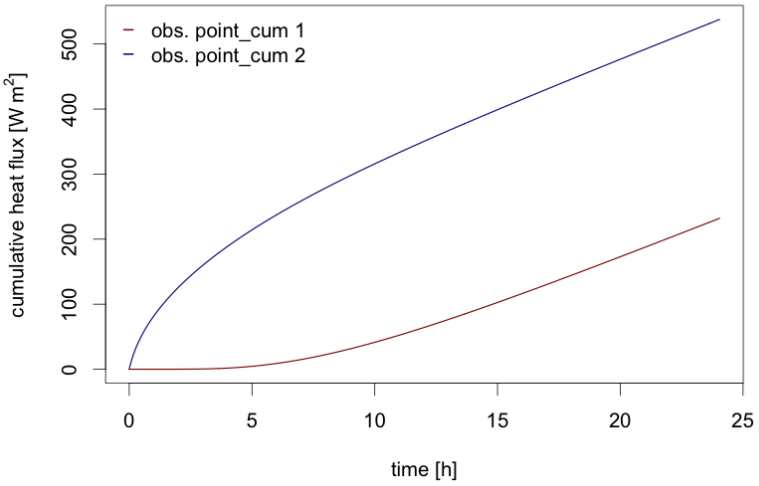


Figure 2.13: Cumulated heat flux at observation points 1 and 2 for a wall with a 15 cm outer stone concrete layer and an inner 5 cm cotton fibre layer generated with Rscript heatplots.R

Scenario 2

1. Open *heat.conf* in a text editor of your choice.
2. Swap the order of materials for specific heat capacity and thermal conductivity. Now, the the outer wall layer is made of cotton fibre and the inner layer is made of concrete.
3. Save heat.conf.

Run scenario 2

Run the simulation in the terminal console.

1. Make sure you are in the right directory.
2. To execute *DRUtES*:
   $ bin/drutes
3. After the simulation finishes, to generate png plots execute provided R script:
   $ Rscript drutes.conf/heat/heatplots.R cottonconcrete
4. The output of the simulation can be found in the folder out

Tasks for scenario 2

1. Answer the same questions as for scenario 1. What is different?

Result of scenario 2

Question 1

Figure 2.14 shows the inner concrete layer becomes linear quite quickly, but that the outer cotton fibre layer has not reached linearity after 24 h. Also taking Fig. 2.15

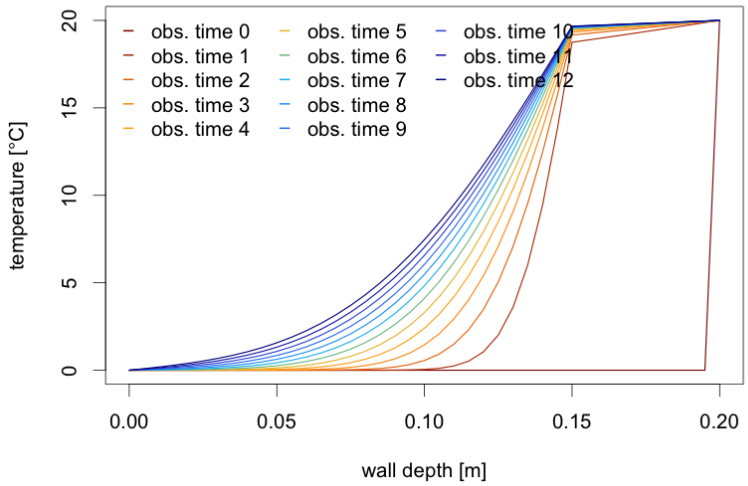


Figure 2.14: Plot of observation times for a wall with a 15 cm thick outer cotton layer and a 5 cm inner concrete stone layer generated with Rscript heatplots.R

Question 2

The system has not reached a constant heat flux, but the heat flux will be between 0.7 and 111 W m^{-2}. A long simulation (not shown) of 240 h shows that the steady state hea flux converges towards 53 W m^{-2}.

Question 3

The cumulative heat flux after 24 h at the inner boundary is higher than in scenario 1, namely 797 W m^{-2}. With a wall area of 15 m^2 this results in $Q = 797$ W h $m^{-2} \cdot 15$ $m^2 = 11955$ W h. For the next 24 h, the heat flux will not be constant and needs to be numerically simulated.

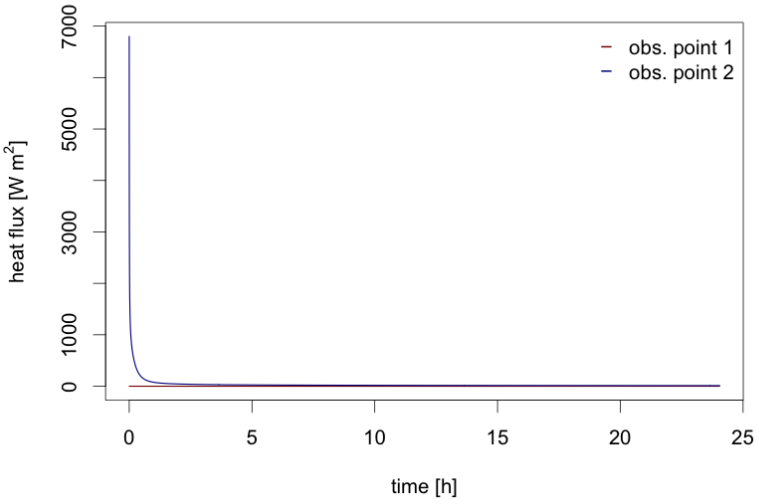


Figure 2.15: Heat flux at observation points for a wall with a 15 cm thick outer cotton layer and a 5 cm inner concrete stone layer generated with Rscript heatplots.R

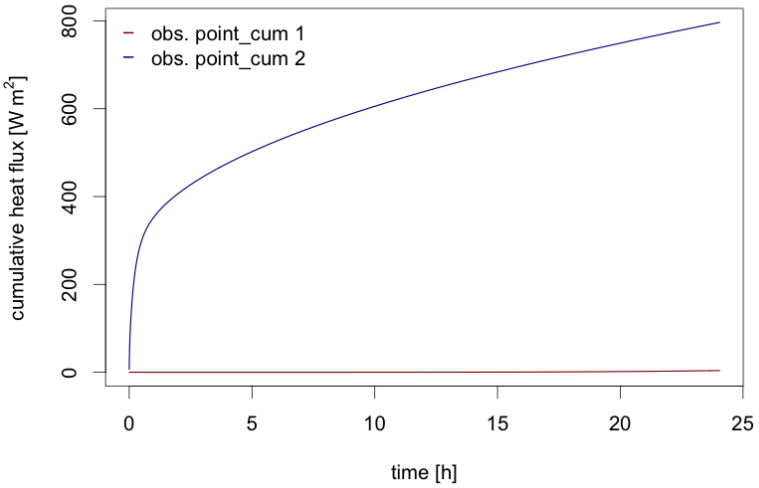


Figure 2.16: Cumulated heat flux at observation points for a wall with a 15 cm thick outer cotton layer and a 5 cm inner concrete stone layer generated with Rscript heatplots.R

2.2.3 Outcome

1. You got familiar with the *DRUtES* heat module in 1D with 2 layers.

2. You simulated heat conduction through a wall with layered materials.

3. You understand the effects of layering of materials with different heat capacities and thermal conductivities.

4. You understand how layering affects when a system is in *steady state*.

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Chapter 3

Water flow module

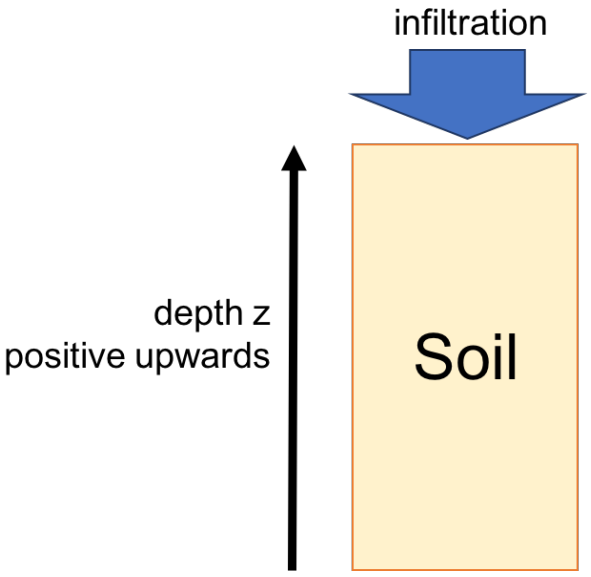
3.1 Infiltration - Part 1

3.1.1 Goal and Complexity

Complexity: Beginner

Prerequisites: None

The goal of this tutorial is to get familiar with the *DRUtES* standard Richards equation module and *DRUtES* configuration in 1D by simulating infiltration into different soil



The process of infiltration is fundamental and yet very important in soil science. Infiltration into the soil determines water, heat and contaminant transport. Infiltration experiments can be used to determine some parameters describing soil hydraulic properties.

In this tutorial three configuration files will be modified step by step. All configuration files are located in the folder *drutes.conf* and respective subfolders.

1. For selection of the module, dimension and time information we require *global.conf*. *global.conf* is located in *drutes.conf / global.conf*.

2. To define the mesh or spatial discretization in 1D, we require *drumesh1D.conf*. *drumesh1D.conf* is located in *drutes.conf / mesh / drumesh1D.conf*.

3. To define the infiltration, we require *matrix.conf*. *matrix.conf* is located in *drutes.conf /water.conf/ matrix.conf*.

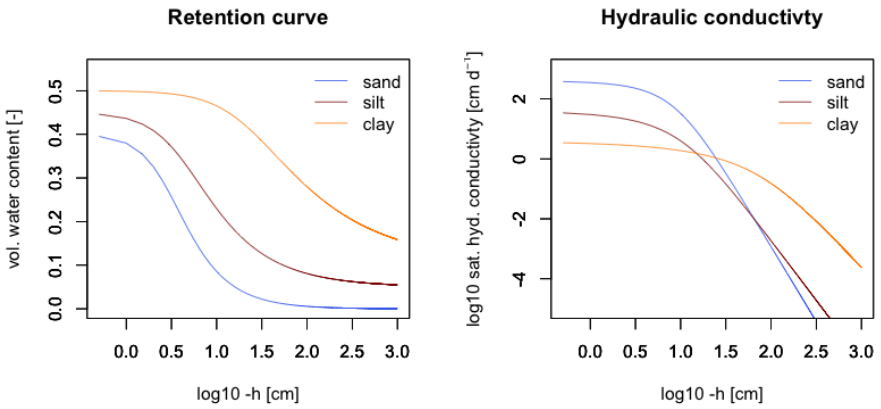
DRUtES works with configuration input file with the file extension .conf. Blank lines and lines starting with # are ignored. The input mentioned in this tutorial therefore needs to be placed one line below the mentioned keyword, unless stated otherwise.

3.1.2 Scenarios

We are using the well-known van Genuchten-Mualem parameterization to describe the soil hydraulic properties of our soils. The parameters describe clay, silt and sand (Tab. 3.1). We assume a constant flow of water infiltrating over the top boundary. We can also look at this as a constant rate of water and it therefore describes the temporal derivative. This type of boundary is called a **Neumann condition**. We assume that the groundwater table is at the bottom of our profile. We therefore assume a constant state of saturation at the bottom profile. In these scenarios we want to investigate the effect of spatial and temporal discretization.

Table 3.1: Material properties needed for scenarios.

Parameter	Description	Sand	Silt	Clay
α [cm^{-1}]	inverse of the air entry value	0.10	0.08	0.01
n [-]	shape parameter	2.2	1.8	1.5
m [-]	shape parameter	0.55	0.44	0.33
θ_s [-]	saturated vol. water content	0.4	0.45	0.5
θ_r [-]	residual vol. water content	0.0	0.05	0.1
Ss [cm^{-1}]	specific storage	1e-9	1e-9	1e-10
K_s [cm d^{-1}]	saturated hydraulic conductivity	400	40	4



Scenario 1

Infiltration into sandy soil.

global.conf: Choose correct model, dimension, time discretization and observation times.

1. Open ***global.conf*** in a text editor of your choice.
2. Model type: Your first input is the module. Input is **RE**.
3. Initial mesh configuration
   (a) The dimension of our problem is 1. Input: 1.
   (b) We use the internal mesh generator. Input: 1.
4. Error criterion
   (a) Maximum number of iteration of the Picard method: 20.
   (b) h tolerance: 1e-1.
5. Time information
   (a) Time units are in hours: input d.
   (b) Initial time: 1e-4.
   (c) End time: 1.
   (d) Minimum time step: 1e-4.
   (e) Maximum time step: 0.1.
6. Observation time settings
   (a) Observation time method: 2.
   (b) Set file format of observation: pure. Output in 1D is always in raw data. Different options will not impact output in 1D.
   (c) Make sequence of observation time: n.
   (d) Number of observation times: 10.

(e) Observation time values: 0.001, 0.005, 0.01, 0.05, 0.1, 0.2, 0.3, 0.4, 0.6, 0.8. Use a new line for each input. *DRUtES* automatically generates output for the initial time and final time. DRUtES will generate 12 output files, e.g. *RE_matrix_press_head-x.dat*, *RE_matrix_theta-x.dat* where x is the number of the file and not the output time. The initial time is assigned an x value of 0.

7. Observation point settings

   (a) Observation point coordinates: 0, 200. Use a new line for each input. *DRUtES* will generate 2 output files, e.g. *obspt_RE_matrix-1.out*, where x is the ID of the observation point.

8. Ignore other settings for now.

9. Save *global.conf*

*drumesh*1*D.conf*: Mesh definition, i.e. number of materials and spatial discretization

1. Open ***drumesh1D.conf*** in a text editor of your choice.

2. Geometry information: 200 cm - domain length

3. Amount of intervals: 1

4.

density	bottom	top
5	0	200

5. Number of materials: 1

6.

id	bottom	top
5	0	200

matrix.conf: Configuration file for water flow

1. Open *matrix.conf* in a text editor of your choice.

2. How-to use constitutive relations? [integer]: 1

3. Length of interval for precalculating the constitutive functions: 200

4. Discretization step for constituitive function precalculation: 0.1

5. Number of soil layers [integer]: 1

6.

alpha	n	m	theta_r	theta_s	specific storage
0.1	2.2	0.55	0.00	0.40	1e-9

7. The angle of the anistropy determines the angle of the reference coordinate system. 0 means vertical flow. Anisothpropy description. Anisothpropy description and hydraulic conductivity

angle [degrees]	K_11
0	400

8. sink(-) /source (+) term per layer: 0

9.

init. cond [real]	type of init. cond	RCZA method [y/n]	RCZA method val.
0.0	H_tot	n	0

10. number of boundaries: 2

11.

boundary ID	boundary type	use rain.dat [y/n]	value
101	1	n	0.0
102	2	n	4

12. Save matrix.conf.

Run scenario 1

Run the simulation in the terminal console.

1. Make sure you are in the right directory.

2. To execute *DRUtES*:

   $ bin/drutes

3. After the simulation finishes, to generate png plots execute provided R script:

   $ Rscript drutes.conf/water.conf/waterplots.R -name sand

4. The output of the simulation can be found in the folder out

Scenario 2

Infiltration into silty soil

1. *global.conf* and *drumesh1D.conf* remain the same.
2. Open *matrix.conf* in a text editor of your choice.
3. Use the same set-up, but change the van Genuchten parameters to:
4.

alpha	n	m	theta_r	theta_s	specific storage
0.08	1.8	0.44	0.05	0.45	1e-9

5. anisothprophy description and hydraulic conductivity

angle [degrees]	K_11
0	40

6. Save matrix.conf.

Run scenario 2

Run the simulation in the terminal console.

1. To execute *DRUtES*:

   $ bin/drutes

2. generate png plots with R script:

   $ Rscript drutes.conf/water.conf/waterplots.R -name silt

Scenario 3

Infiltration into clay soil

1. *global.conf* and *drumesh1D.conf* remain the same.
2. Open *matrix.conf* in a text editor of your choice.
3. Use the same set-up, but change the van Genuchten parameters to:

4.

alpha	n	m	theta_r	theta_s	specific storage
0.01	1.5	0.33	0.1	0.5	1e-10

5. anisothprophy description and hydraulic conductivity

angle [degrees]	K_11
0	4

6. Save matrix.conf.

Run scenario 3

Run the simulation in the terminal console.

1. To execute *DRUtES*:
   $ bin/drutes

2. generate png plots with R script:
   $ Rscript drutes.conf/water.conf/waterplots.R -name clay

Tasks

1. Describe the infiltration fronts for sand, silt and clay.

2. The results of the fluxes look horrible. This is because of insufficient discretization. Improve the discretization. With what set-up are the results better? Possibilities are:

   - in global.conf: Decrease the pressure head tolerance, Decrease the initial time step, Decrease the maximum time step.
   - in drumesh1D.conf: Decrease the mesh density.

Results

In the following time series of the infiltration into sand, silt and clay are presented. The infiltration front has moved furthest in clay, followed by sand and then silt. However, the time series show that their numerical approximation is insufficient, especially for sand. This is

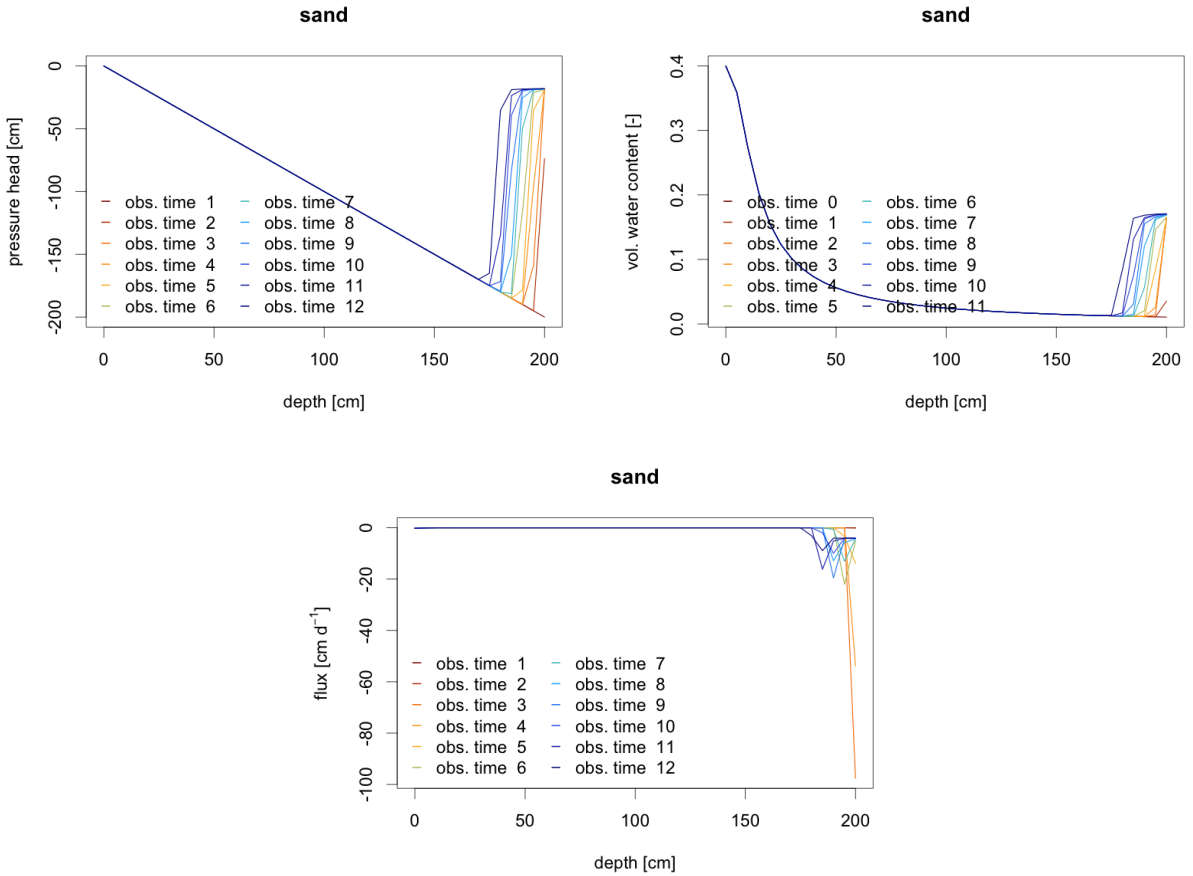


Figure 3.1: Observation time series of pressure head, vol. water content and flux of infiltration into sand.

because sand is the numerically most difficult to model as it has the steepest retention properties (largest n and largest alpha). In the beginning, the flux in sand is 100 cm d^{-1}, which is 20 times the size of the assigned flux. For silt, the flux is overestimated approximately 12 times and for clay, the flux is overestimated twice.

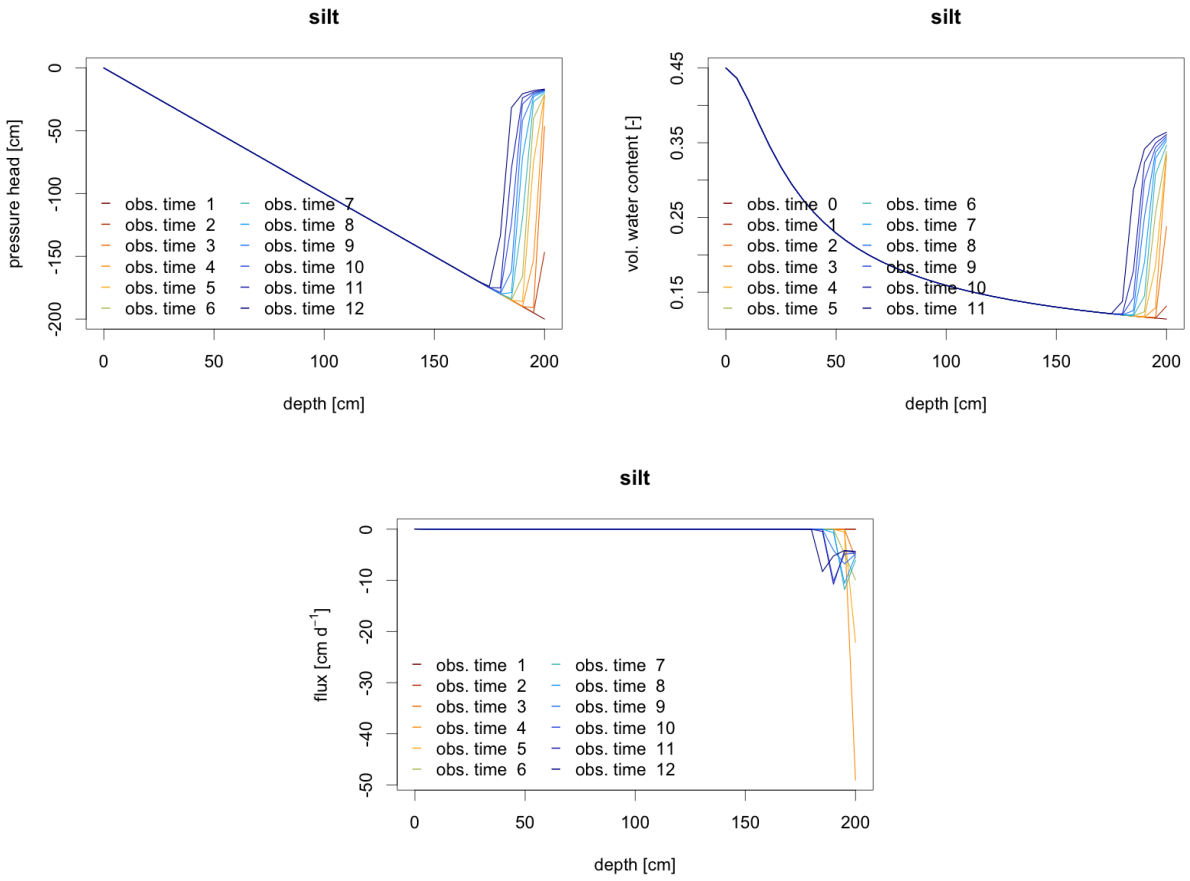


Figure 3.2: Observation time series of pressure head, vol. water content and flux of infiltration into silt.

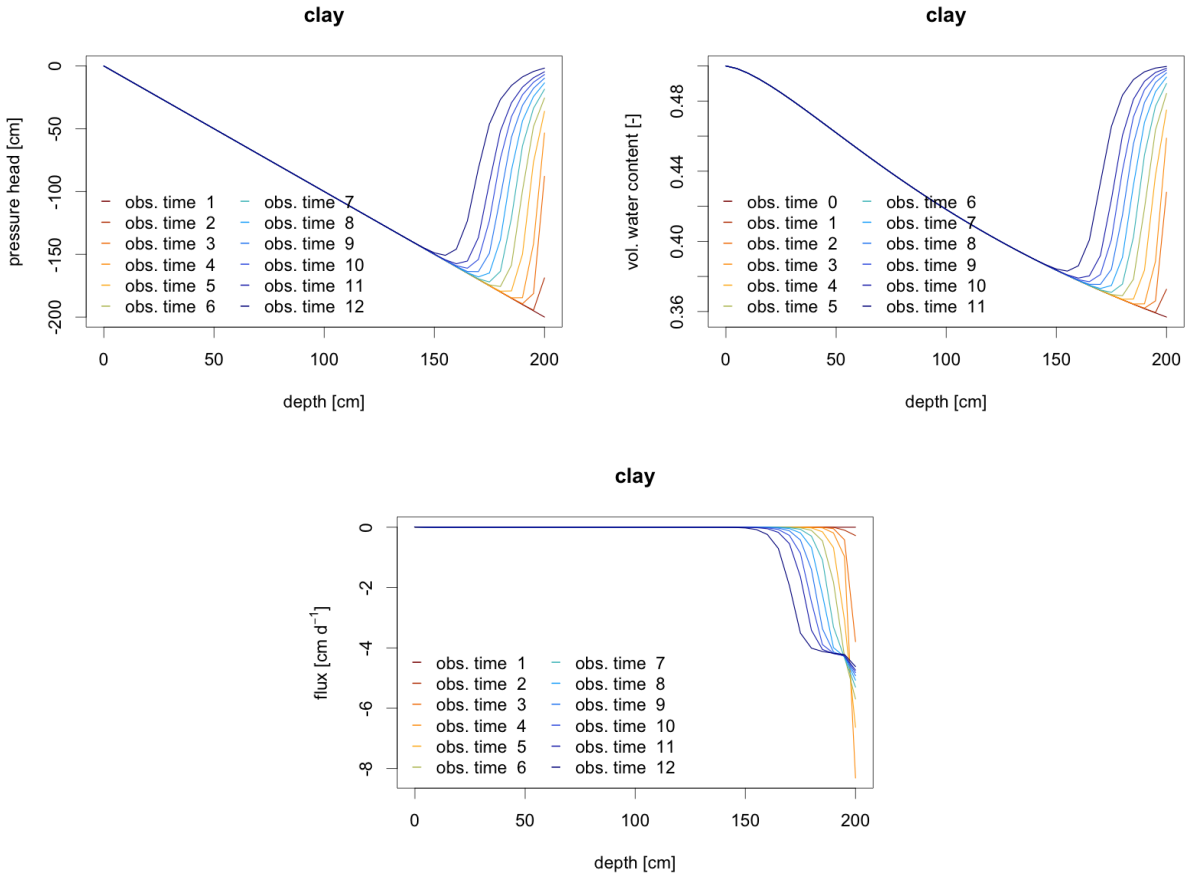


Figure 3.3: Observation time series of pressure head, vol. water content and flux of infiltration into clay.

3.1.3 Outcome

1. You got familiar with the *DRUtES* standard Richards Equation modules in 1D.
2. You understand basic parameterization of a typical sand, silt and clay with the van Genuchten-Mualem model.
3. You simulated infiltration in different soils.
4. You understand the term *Neumann boundary condition* and *initial condition.*
5. You understand the effects of different discretizations.

3.2 Infiltration - Part 2

3.2.1 Goal and Complexity

Complexity: Beginner

Prerequisites: None

The goal of this tutorial is to get familiar with the *DRUtES* standard Richards equation module and *DRUtES* configuration in 1D by simulating infiltration into different soil

3.2.2 Scenarios

We use the same parameters as in the previous infiltration scenario (Tab. 3.1). We assume a constant ponding depth at the top boundary. Similar to the state of saturation in the previous scenario at the bottom boundary, where we knew the solution of the water table, we can assume the height of the water table, the ponding depth, to be defined with a Dirichlet condition, where the value is similar to the height of the ponding depth. At the bottom, we assume that only gravitational force acts on the bottom drainage. This also means that the pressure head gradient is zero. This boundary condition is called **free drainage**. The set-up of these scenarios are the same as in the previous infiltration scenarios, except

for the boundary conditions. In these scenarios, we also want to investigate the effects on discretization, especially on the flux over the top boundary.

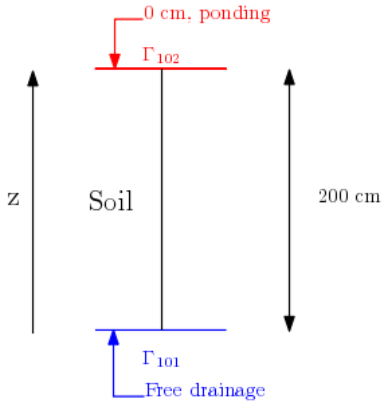


Figure 3.4: 1D domain set-up of infiltration scenario with top and bottom boundary conditions. A constant ponding is assigned to the top, defined with a Dirichlet condition of 0 cm. Free drainage occurs at the bottom, which indicates that the pressure head gradient is 0 and water flows only due to gravity.

Scenario 1

Infiltration into sandy soil.

global.conf: Choose correct model, dimension, time discretization and observation times.

1. Open ***global.conf*** in a text editor of your choice.
2. Model type: Your first input is the module. Input is **RE**.
3. Initial mesh configuration
   (a) The dimension of our problem is 1. Input: 1.
   (b) We use the internal mesh generator. Input: 1.
4. Error criterion
   (a) Maximum number of iteration of the Picard method: 20
   (b) h tolerance: 1e-1.
5. Time information
   (a) Time units are in hours: input d
   (b) Initial time: 1e-4.
   (c) End time: 1.
   (d) Minimum time step: 1e-4.
   (e) Maximum time step: 0.1.
6. Observation time settings
   (a) Observation time method: 2
   (b) Set file format of observation: pure. Output in 1D is always in raw data. Different options will not impact output in 1D.
   (c) Make sequence of observation time: n
   (d) Number of observation times: 10

(e) Observation time values: 0.001, 0.005, 0.01, 0.05, 0.1, 0.2, 0.3, 0.4, 0.6, 0.8. Use a new line for each input. *DRUtES* automatically generates output for the initial time and final time. DRUtES will generate 12 output files, e.g. *RE_matrix_press_head-x.dat*, *RE_matrix_theta-x.dat* where x is the number of the file and not the output time. The initial time is assigned an x value of 0.

7. Observation point settings

   (a) Observation point coordinates: 0, 200. Use a new line for each input. *DRUtES* will generate 2 output files, e.g. *obspt_RE_matrix-1.out*, where x is the ID of the observation point.

8. Ignore other settings for now.

9. Save *global.conf*

*drumesh*1*D.conf*: Mesh definition, i.e. number of materials and spatial discretization

1. Open ***drumesh1D.conf*** in a text editor of your choice.

2. Geometry information: 200 cm - domain length

3. Amount of intervals: 1

4.

density	bottom	top
5	0	200

5. number of materials: 1

6.

id	bottom	top
5	0	200

matrix.conf: Configuration file for water flow

1. Open *matrix.conf* in a text editor of your choice.

2. How-to use constitutive relations? [integer]: 1

3. Length of interval for precalculating the constitutive functions: 200

4. Discretization step for constituitive function precalculation: 0.1

5. number of soil layers [integer]: 1

6.

alpha	n	m	theta_r	theta_s	specific storage
0.1	2.2	0.55	0.00	0.40	0

7. The angle of the anisotropy determines the angle of the reference coordinate system. 0 means vertical flow. Anisotropy description. Anisotpropy description and hydraulic conductivity

angle [degrees]	K_11
0	400

8. sink(-) /source (+) term per layer: 0

9. Initial condition is a constant pressure head of -200 cm across the soil.

init. cond [real]	type of init. cond	RCZA method [y/n]	RCZA method val.
-200.0	hpres	n	0

10. number of boundaries: 2

11.

boundary ID	boundary type	use rain.dat [y/n]	value
101	3	n	0.0
102	1	n	0.0

12. Save matrix.conf.

Run scenario 1

Run the simulation in the terminal console.

1. Make sure you are in the right directory.

2. To execute *DRUtES*:

   $ bin/drutes

3. After the simulation finishes, to generate png plots execute provided R script:

   $ Rscript drutes.conf/water.conf/waterplots.R -name sand

4. The output of the simulation can be found in the folder out

Scenario 2

Infiltration into silty soil

1. *global.conf* and *drumesh1D.conf* remain the same.
2. Open *matrix.conf* in a text editor of your choice.
3. Use the same set-up, but change the van Genuchten parameters to:
4.

alpha	n	m	theta_r	theta_s	specific storage
0.08	1.8	0.44	0.05	0.45	0

5. anisothprophy description and hydraulic conductivity

angle [degrees]	K_11
0	40

6. Save matrix.conf.

Run scenario 2

Run the simulation in the terminal console.

1. To execute *DRUtES*:

   $ bin/drutes

2. generate png plots with R script:

   $ Rscript drutes.conf/water.conf/waterplots.R -name silt

Scenario 3

Infiltration into clay soil

1. *global.conf* and *drumesh1D.conf* remain the same.
2. Open *matrix.conf* in a text editor of your choice.
3. Use the same set-up, but change the van Genuchten parameters to:

4.

alpha	n	m	theta_r	theta_s	specific storage
0.01	1.5	0.33	0.1	0.5	0

5. anisothprophy description and hydraulic conductivity

angle [degrees]	K_11
0	4

6. Save matrix.conf.

Run scenario 3

Run the simulation in the terminal console.

1. To execute *DRUtES*:
   $ bin/drutes

2. generate png plots with R script:
   $ Rscript drutes.conf/water.conf/waterplots.R -name clay

Tasks

1. Describe the infiltration fronts for sand, silt and clay.

2. The results do not look very smooth. This is because of insufficient discretization. Improve the discretization for sand. With what set-up are the results better? Possibilities are:

   - in global.conf: Decrease the pressure head tolerance, Decrease the initial time step, Decrease the maximum time step.
   - in drumesh1D.conf: Decrease the mesh density.

3. Why is the flux at the top so huge in the beginning?

Results

Task 1

In the following time series of the infiltration into sand, silt and clay are presented. The infiltration front has moved furthest in sand, followed by silt and then clay. This is because of the assigned boundary conditions. The flux into sandy soil is very large. However, the time series show the numerical approximation is insufficient, especially for sand. This is because sand is the numerically most difficult to model as it has the steepest retention properties (largest n and largest alpha).

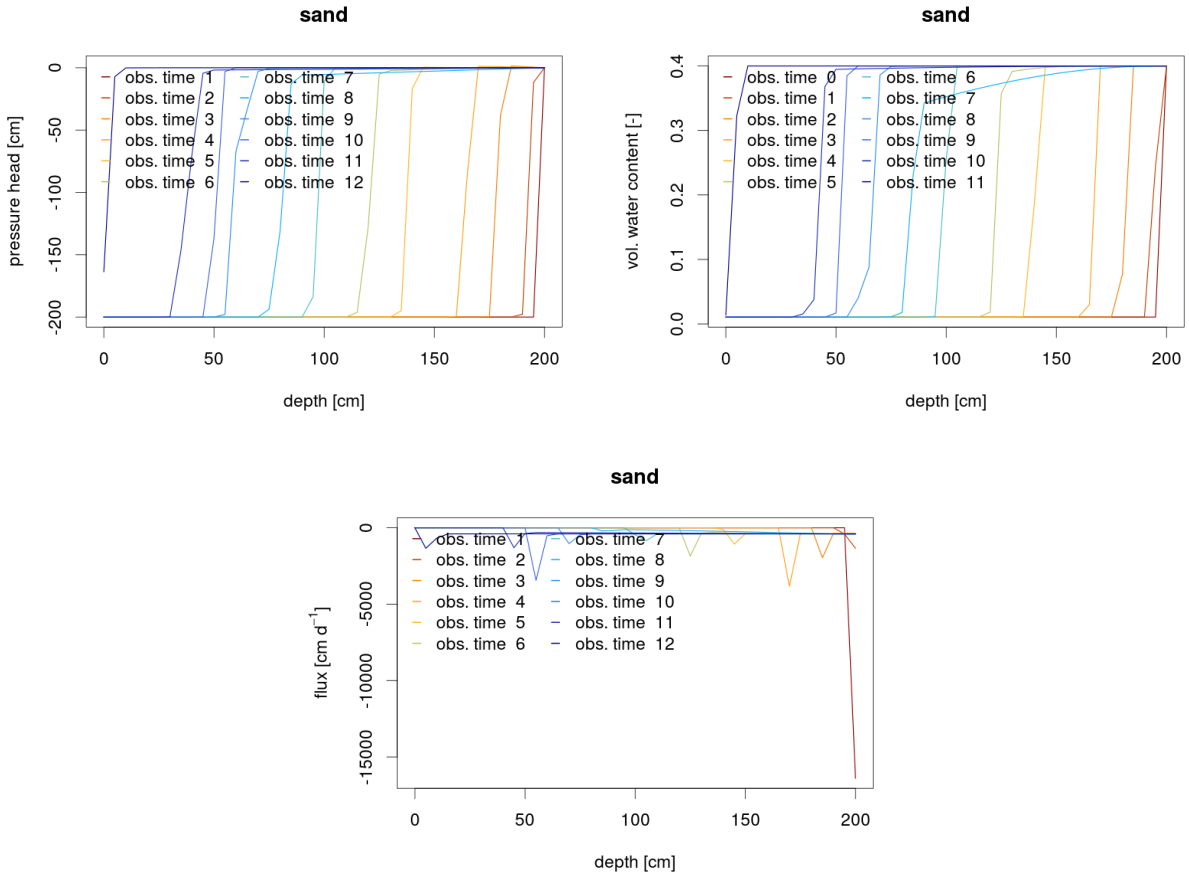


Figure 3.5: Observation time series of pressure head, vol. water content and flux of infiltration into sand.

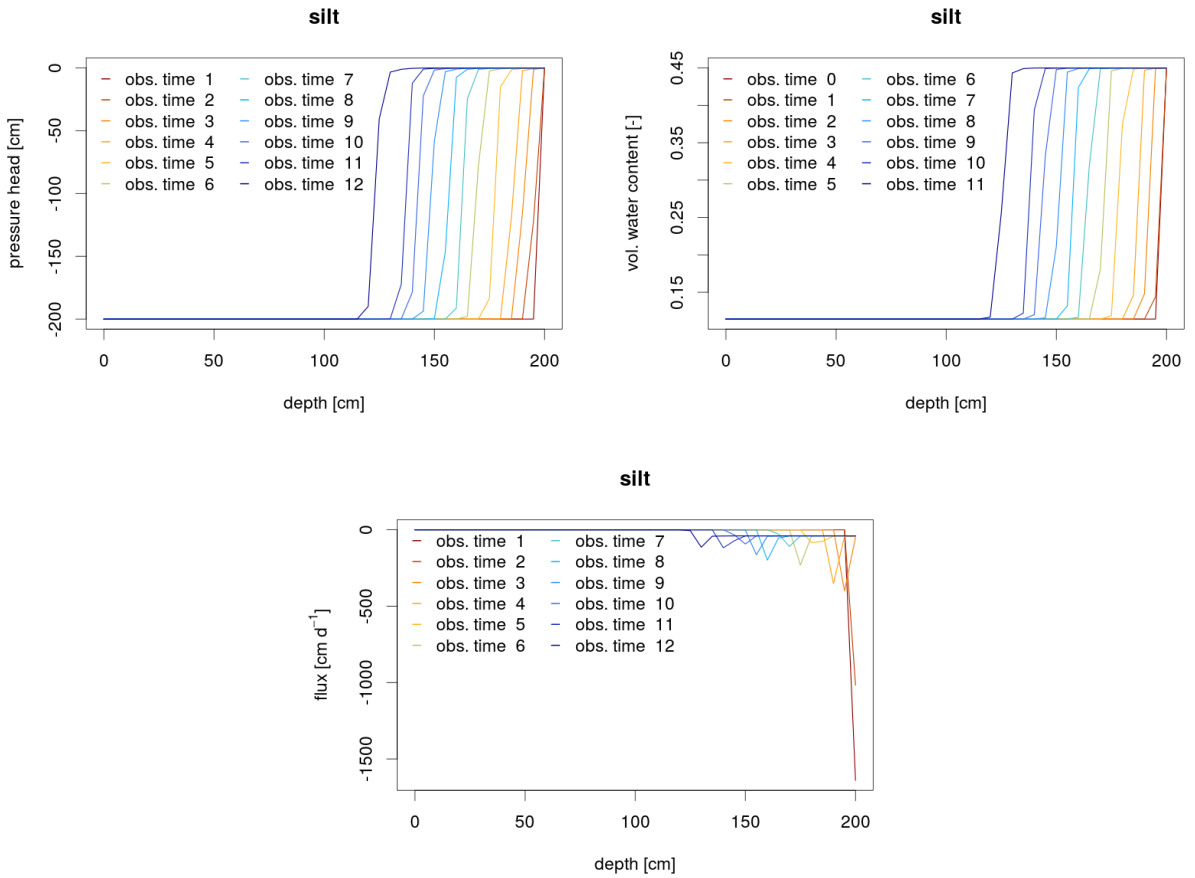


Figure 3.6: Observation time series of pressure head, vol. water content and flux of infiltration into silt.

Task 2

The solution for sand the water content and hydraulic pressure become a lot smoother with finer spatial discretization, eg. dz=0.5 and a finer temporal discretization by setting the lower minimal time step to 0.01. The fluxes are still spiky, but correlate with the infiltration front. Different solutions can be found by decreasing the minimal time step even further and also the h tolerance criterion. This, however, increases the simulation time substantially. For a reliable solution, the numerical solution should converge. This means that decreasing the time step, or discretization, should not lead to an entirely different solution. We notice, that reducing the h tolerance criterion improves the solution locally, but that reducing the maximum time step changes the depth of the infiltration front. This is because the mass balance is very much connected to the temporal discretization.

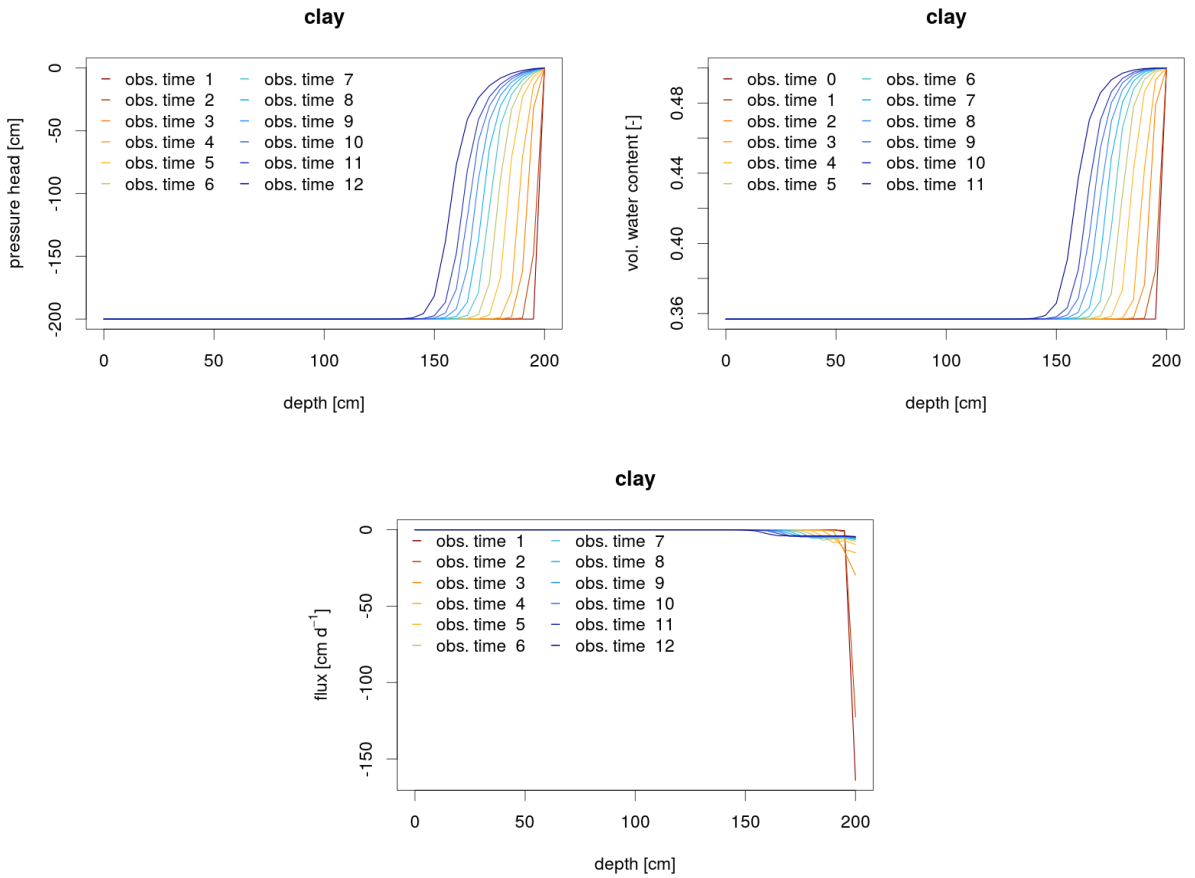


Figure 3.7: Observation time series of pressure head, vol. water content and flux of infiltration into clay.

Task 3

With the initial set-up, the flux at the top in sand is 15000 cm d^{-1} in the beginning of the simulation. For silt, the flux was numerically calculated to be at 1500 cm d^{-1} and for clay at 150 cm d^{-1}. The flux estimation becomes a lot larger with finer spatial discretization.

This is due to the large hydraulic gradient between the saturated top boundary and the next node of $\nabla h = \frac{-200-0}{\mathrm{dz}}$. The smaller the nodal distance dz is, the greater is the gradient. According to the Darcy-Buckingham law, the flux is proportional to the hydraulic conductivity. The hydraulic conductivity is highest for sand. This is why the flux is largest for sand and lowest for clay.

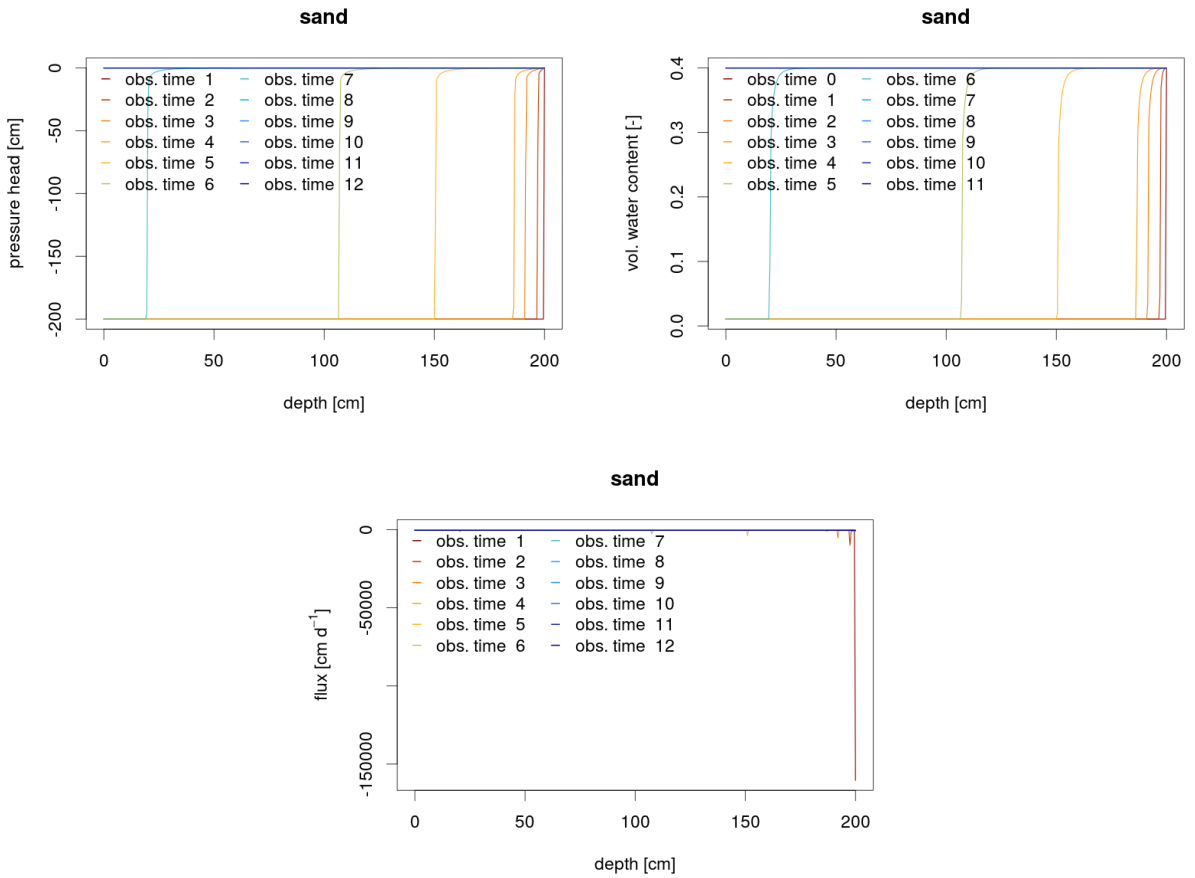


Figure 3.8: Observation time series of pressure head, vol. water content and flux of infiltration into sand with improved discretization.

3.2.3 Outcome

1. You got familiar with the *DRUtES* standard Richards Equation modules in 1D.
2. You understand basic parameterization of a typical sand, silt and clay with the van Genuchten-Mualem model.
3. You simulated infiltration in different soils.
4. You understand the term *Free drainage* and *initial condition*.
5. You understand the effects of different discretizations.

Chapter 4

Coupled models

4.1 Coupled water and heat flow

4.1.1 Goal and Complexity

Complexity: Medium

Prerequisites: Heat and Water Flow

The goal of this tutorial is to get familiar with the idea of coupled models in 1D. For this we couple the *DRUtES* standard Richards equation module and the heat module. We apply solar radiation data and rain and evaporation data as input.

In the real world many coupled processes occur. In our model, heat conduction is dependent on the water flow as it transports the heat in the soil. In reality, heat and water is even more closely coupled as soil hydraulic properties are also dependent on temperature, e.g. surface tension and density change with temperature.

In this tutorial three configuration files will be modified step by step. All configuration files are located in the folder *drutes.conf* and respective subfolders.

1. For selection of the module, dimension and time information we require *global.conf*. *global.conf* is located in *drutes.conf / global.conf*.

2. To define the mesh or spatial discretization in 1D, we require *drumesh1D.conf*. *drumesh1D.conf*

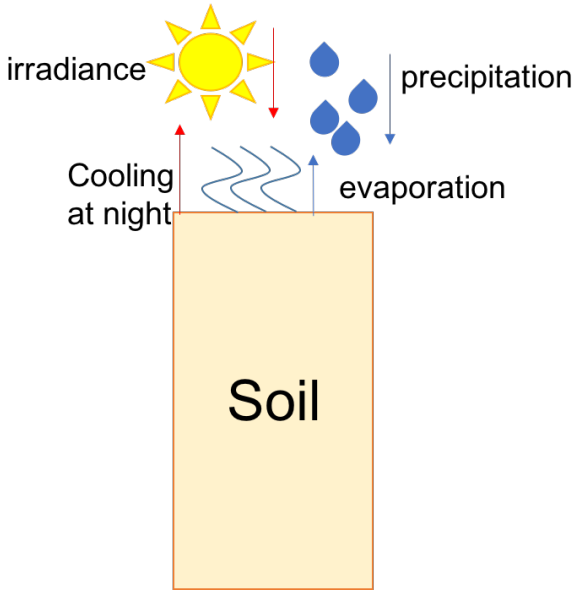


Figure 4.1: Simplified scheme of coupled model.

is located in *drutes.conf / mesh / drumesh1D.conf*.

3. To define the radiation and cooling, we require *heat.conf*. *heat.conf* is located in *drutes.conf /heat/ heat.conf*.

4. To define the precipitation and evaporation, we require *matrix.conf*. *matrix.conf* is located in *drutes.conf /water.conf/ matrix.conf*.

DRUtES works with configuration input file with the file extension .conf. Blank lines and lines starting with # are ignored. The input mentioned in this tutorial therefore needs to be placed one line below the mentioned keyword, unless stated otherwise.

4.1.2 Scenarios

For these coupled scenarios we need to define four boundary conditions, two for the heat flow and two for the water flow. We assume simplifying conditions for the bottom boundary. We assume the groundwater table to be at the bottom boundary. This condition does not change over time. Therefore we assign a constant Dirichlet condition for the water flow. We also assume that the temperature of the groundwater remains constant for the given simulation time. This means that we know the temperature, the solution of the heat flow equation and therefore assign a Dirichlet condition for the heat flow.

In the following scenarios, the water flow is determined by evaporation and precipitation, or more generally time-varying rates of water, therefore the top boundary for the water flow is a Neumann condition. The heat flow over the top boundary is determined by radiation by the sun during the day and radiative cooling during the night. This condition can be understood as a Neumann condition. In these scenarios we want to investigate patterns of temperature oscillations.

We use time-varying boundary conditions for the heat and water flow, which need to be read from files. The file meteo_heat.bc needs to be renamed to 102.bc in the heat folder. The file meteo_water.bc needs to be renamed to 102.bc in the water.conf folder.

The material properties needed for scenarios are in Tab. 4.1.

Table 4.1: Material properties needed for scenarios.

Parameter	Description	Soil
α [cm^{-1}]	inverse of the air entry value	0.05
n [-]	shape parameter	2
m [-]	shape parameter	0.5
θ_s [-]	saturated vol. water content	0.45
θ_r [-]	residual vol. water content	0.05
Ss [cm^{-1}]	specific storage	0
K_s [cm d^{-1}]	saturated hydraulic conductivity	100
c_l [Wd cm^{-3} K^{-1}]	specific heat capacity of soil	2.545e-5
c_w [Wd cm^{-3} K^{-1}]	specific heat capacity of water	4.843e-5
λ [W cm^{-1} K^{-1}]	thermal conductivity	0.02

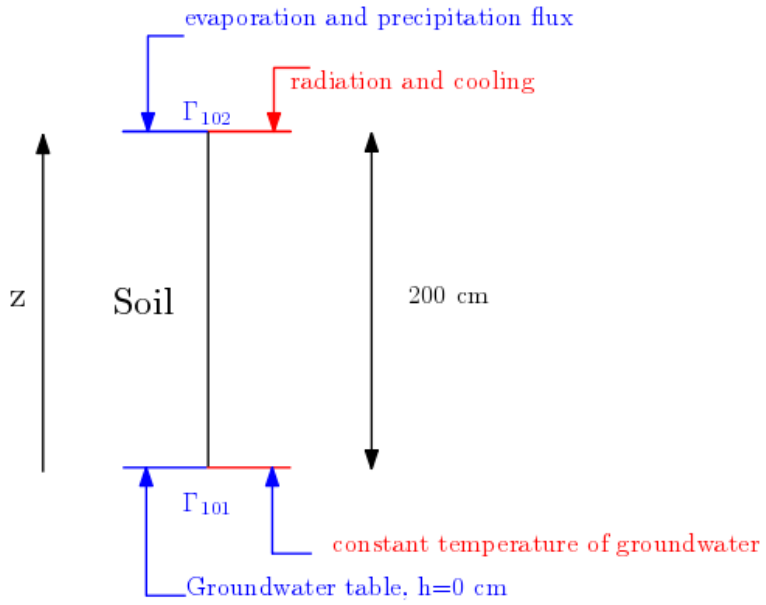


Figure 4.2: 1D domain set-up of coupled scenario with top and bottom boundary conditions. There are now two boundary condtions at the top and two boundary conditions at the bottom: heat and water flow. The top boundary is defined by the interactions with the atmosphere and the bottom boundary is defined by the constant groundwater table.

Scenario 1

Coupled model

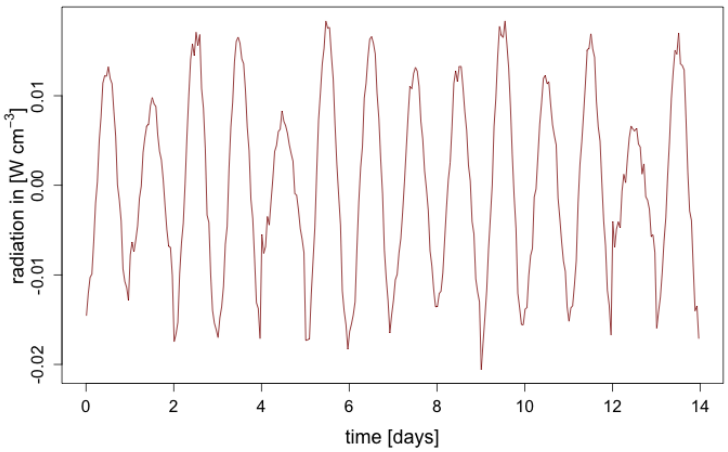


Figure 4.3: Heat flow data used for the top boundary

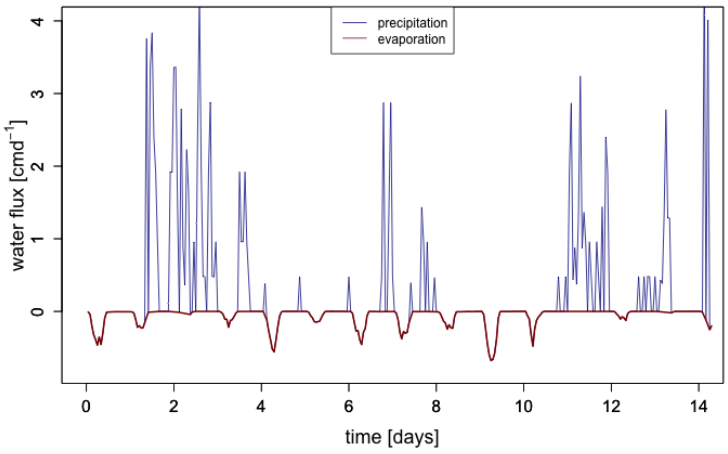


Figure 4.4: Water flow data used for the top boundary

global.conf: Choose correct model, dimension, time discretization and observation times.

1. Open ***global.conf*** in a text editor of your choice.

2. Model type: Your first input is the module. Input is **heat**.

3. Initial mesh configuration

   (a) The dimension of our problem is 1. Input: 1.

   (b) We use the internal mesh generator. Input: 1.

4. Error criterion
   (a) Maximum number of iteration of the Picard method: 20
   (b) h tolerance: 1.
5. Time information
   (a) Time units are in hours: input d
   (b) Initial time: 1e-6.
   (c) End time: 14.
   (d) Minimum time step: 1e-6.
   (e) Maximum time step: 0.001.
6. Observation time settings
   (a) Observation time method: 2
   (b) Set file format of observation: pure. Output in 1D is always in raw data. Different options will not impact output in 1D.
   (c) Make sequence of observation time: n
   (d) Number of observation times: 0
   (e) Observation time values: #
7. Observation point settings
   (a) Number of observation points: 6
   (b) Observation point coordinates: 200, 195,180,160,140, 120. Use a new line for each input. *DRUtES* will generate 6 output files, e.g. *obspt_RE_matrix-1.out*, where x is the ID of the observation point.
8. Ignore other settings for now.
9. Save $global.conf$

$drumesh1D.conf$: Mesh definition, i.e. number of materials and spatial discretization

1. Open ***drumesh1D.conf*** in a text editor of your choice.

2. Geometry information: 200 cm - domain length

3. Amount of intervals: 1

4.

density	bottom	top
4	0	200

5. number of materials: 1

6.

id	bottom	top
1	0	200

matrix.conf: Configuration file for water flow

1. Open *matrix.conf* in a text editor of your choice.

2. How-to use constitutive relations? [integer]: 1

3. Length of interval for precalculating the constitutive functions: 200

4. Discretization step for constituitive function precalculation: 0.1

5. number of soil layers [integer]: 1

6.

alpha	n	m	theta_r	theta_s	specific storage
0.05	2	0.5	0.05	0.45	0

7. The angle of the anisotropy determines the angle of the reference coordinate system. 0 means vertical flow. Anisotropy description. Anisotpropy description and hydraulic conductivity

angle [degrees]	K_11
0	100

8. sink(-) /source (+) term per layer: 0

9. Initial condition is a constant pressure head of -200 cm across the soil.

init. cond [real]	type of init. cond	RCZA method [y/n]	RCZA method val.
0.0	H_tot	n	0

10. number of boundaries: 2

11.

boundary ID	boundary type	use rain.dat [y/n]	value
101	1	n	0.0
102	2	y	0.0

12. Save matrix.conf.

heat.conf: Heat module after Sophocleous (1979).

1. Open *heat.conf* in a text editor of your choice.
2. Couple with Richards equation: y
3. Number of materials or layers: 1
4. Specific heat capacity of the wall material: 2.545e-5 Wd cm^{-3} K^{-1}
5. Specific heat capacity of liquid: 4.843e-5 Wd cm^{-3} K^{-1}
6. Anisotropy: There is no anisotropy. The value is 0.
7. Heat conductivity of the soil material: 0.02 W cm^{-1} K^{-1}.
8. There is NO heat convection of water: 0.
9. The initial temperature is 0°C across the entire domain: 0.
10. There is no heat source: 0.
11. We have 2 boundaries at top and bottom of the soil column. We assume a constant temperature of 15 °C at the bottom where the groundwater table is. We assume the the top to be influenced by radiation and cooling, which are both flux or Neumann conditions.

boundary id	boundary type	use bc.dat	value
101	1	n	15.0
102	2	y	0.0

12. Save heat.conf.

Run scenario 1

Run the simulation in the terminal console.

1. Make sure you are in the right directory.
2. To execute *DRUtES*:
   $ bin/drutes
3. After the simulation finishes, to generate png plots execute provided R script:
   $ Rscript drutes.conf/water.conf/waterplots.R -name coupled
   $ Rscript drutes.conf/heat/heatplots.R coupled
4. The output of the simulation can be found in the folder out

Tasks

1. Describe the temperature and water content distribution.

Results

The water content at the top follows the flux input. The lower the observation point, the less fluctuations can be observed. The temperature follows the heat flux input. The temperature fluctuations become smaller with depth, but also show a lag time.

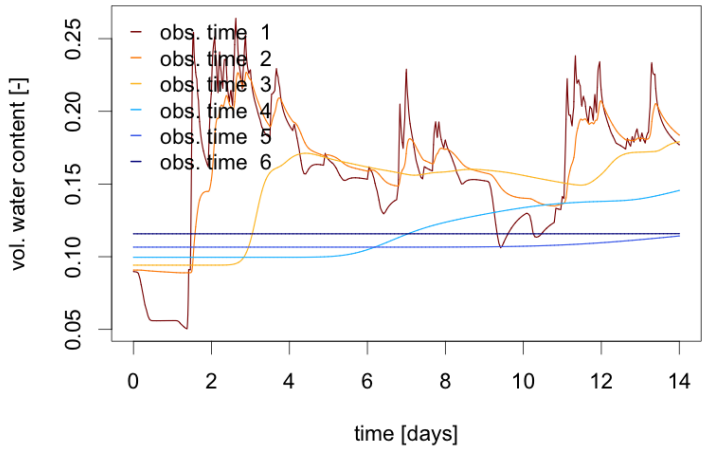


Figure 4.5: Water content at the observation points

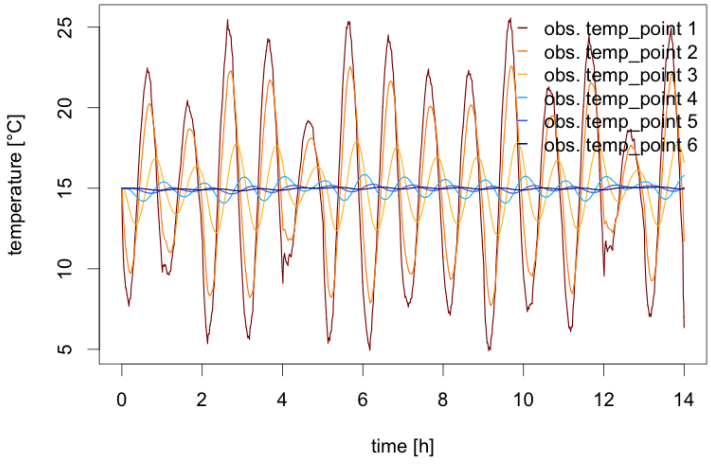


Figure 4.6: Temperature at the observation points.

4.1.3 Outcome

1. You got familiar with the idea of coupled models.
2. You simulated coupled water flow and heat flow.
3. You understand the influence of distance to input flux and how the top is the most varying layer.

4.2 Coupled water flow and contaminant transport

4.2.1 Goal and Complexity

Complexity: Medium

Prerequisites: Water flow module

The goal of this tutorial is to introduce contaminant transport. For this we couple the *DRUtES* standard Richards equation module with the ADE module. ADE stands for Advection-Dispersion-Equation. The advection will be calculated through the Richards-Equation (water flow).

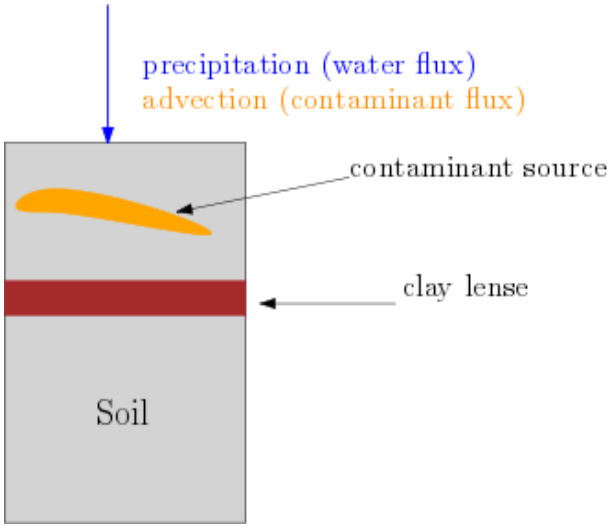


Figure 4.7: Simplified scheme of coupled model.

In this example we assume that the contaminant is soluble and in the water. No adsorption or desorption occurs.

In this tutorial five configuration files will be modified step by step. All configuration files are located in the folder *drutes.conf* and respective subfolders.

1. For selection of the module, dimension and time information we require *global.conf*. *global.conf* is located in *drutes.conf* / *global.conf*.

2. To define the mesh or spatial discretization in 1D, we require *drumesh1D.conf*. *drumesh1D.conf* is located in *drutes.conf* / *mesh* / *drumesh1D.conf*.

3. To define the precipitation, we require *matrix.conf*. *matrix.conf* is located in *drutes.conf /water.conf/ matrix.conf*.

4. To select the ADE module and link it to the water module, we require *ADE.conf*. *ADE.conf* is located in *drutes.conf /ADE/ ADE.conf*.

5. To define the contaminant transport, we require *contaminant.conf*. *contaminant.conf* is located in *drutes.conf /ADE/ contaminant.conf*.

DRUtES works with configuration input file with the file extension .conf. Blank lines and lines starting with # are ignored. The input mentioned in this tutorial therefore needs to be placed one line below the mentioned keyword, unless stated otherwise.

4.2.2 Scenarios

In the following scenario, there is a contaminant of a known concentration in the soil, which we can set with appropriate layering of our domain and the initial condition. This coupled model also requires four boundary conditions, two for the water flow and two for the contaminant transport. We assume that the contaminant does not reach the bottom of our domain, nor the top boundary. The boundary conditions for the contaminant transport at both boundaries are constant Dirichlet conditions. The bottom boundary represents the groundwater table. We assign a Dirichlet condition for the water flow at the bottom of the profile. We assume precipitation occurs at the top boundary and therefore, we assign a Neumann condition at the top boundary. In these scenarios we want to investigate the effect of a soil layer with different hydraulic properties below the contaminant.

Table 4.2: Material properties needed for scenarios.

Parameter	Description	Sand	Clay	Contaminant
α [cm^{-1}]	inverse of the air entry value	0.05	0.01	
n [-]	shape parameter	2	1.4	
m [-]	shape parameter	0.5	0.2857	
θ_s [-]	saturated vol. water content	0.45	0.45	
θ_r [-]	residual vol. water content	0.05	0.05	
Ss [cm^{-1}]	specific storage	0	0	
K_s [cm d^{-1}]	saturated hydraulic conductivity	100	1	
D [cm^2 d^{-1}]	diffusion	10e-3	10e-3	
D_v [cm]	dispersivity	30	100	
c_{init} [mg cm^{-3}]	initial concentration			2

The domain scheme is shown in Fig. 4.8. We need to define 4 boundary conditions. Our mesh requires 5 different layers to accomodate for the contaminantion, the extra soil and the layers in between.

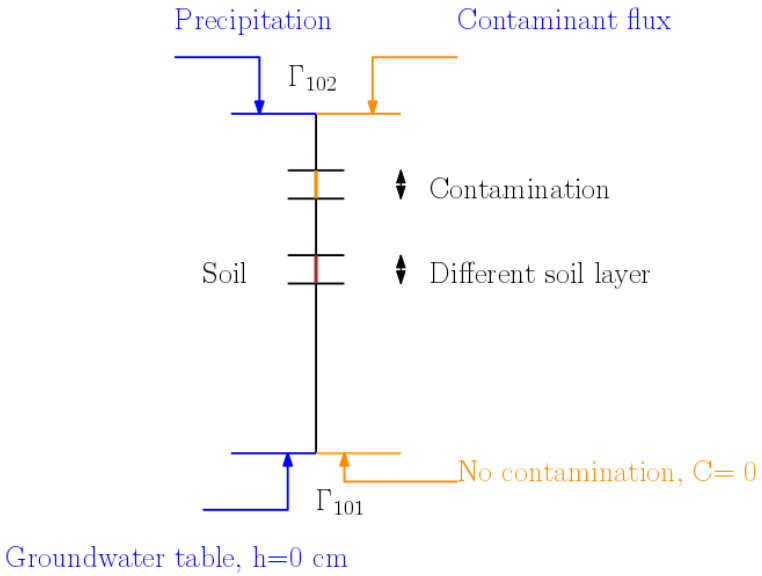


Figure 4.8: 1D domain set-up of coupled scenario with top and bottom boundary conditions. There are now two boundary condtions at the top and two boundary conditions at the bottom: contaminant transport and water flow. The top boundary is defined by the interactions with the atmosphere and the bottom boundary is defined by the constant groundwater table.

Scenario 1

We first assume that the soil is homogeneous.

global.conf: Choose correct model, dimension, time discretization and observation times.

1. Open ***global.conf*** in a text editor of your choice.
2. Model type: Your first input is the module. Input is **ADE**.
3. Initial mesh configuration
   (a) The dimension of our problem is 1. Input: 1.
   (b) We use the internal mesh generator. Input: 1.
4. Error criterion
   (a) Maximum number of iteration of the Picard method: 20
   (b) h tolerance: 1e-3.
5. Time information

(a) Time units are in hours: input d

(b) Initial time: 1e-4.

(c) End time: 10.

(d) Minimum time step: 1e-12.

(e) Maximum time step: 0.005.

6. Observation time settings

(a) Observation time method: 2

(b) Set file format of observation: pure. Output in 1D is always in raw data. Different options will not impact output in 1D.

(c) Make sequence of observation time: n

(d) Number of observation times: 9

(e) Observation time values: 1, 2, 3,4,5,6,7,8,9. Use a new line for each input. *DRUtES* will generate 11 output files for each modeled component, e.g.*RE_ matrix_ press_ hea x.dat*, where x is the ID of the observation point. The initial and final time value will be automatically be printed.

7. Observation point settings

(a) Number of observation points: 6

(b) Observation point coordinates: 200, 195,187.5,182.5,175, 150. Use a new line for each input. *DRUtES* will generate 6 output files for each modeled component, e.g. *obspt_ RE_ matrix-1.out*, where x is the ID of the observation point.

8. Ignore other settings for now.

9. Save *global.conf*

*drumesh*1*D.conf*: Mesh definition, i.e. number of materials and spatial discretization

1. Open ***drumesh1D.conf*** in a text editor of your choice.

2. Geometry information: 200 cm - domain length

3. Amount of intervals: 1

4.

density	bottom	top
4	0	200

5. number of materials: 5

6.

id	bottom	top
1	0	170
2	170	180
3	180	185
4	185	190
5	190	200

7. Save $drumesh1D.conf$

matrix.conf: Configuration file for water flow

1. Open *matrix.conf* in a text editor of your choice.

2. How-to use constitutive relations? [integer]: 1

3. Length of interval for precalculating the constitutive functions: 200

4. Discretization step for constituitive function precalculation: 0.1

5. number of soil layers [integer]: 5

6.

alpha	n	m	theta_r	theta_s	specific storage
0.05	2	0.5	0.05	0.45	0
0.05	2	0.5	0.05	0.45	0
0.05	2	0.5	0.05	0.45	0
0.05	2	0.5	0.05	0.45	0
0.05	2	0.5	0.05	0.45	0

7. The angle of the anisotropy determines the angle of the reference coordinate system. 0 means vertical flow. Anisotropy description. Anisotpropy description and hydraulic

conductivity

angle [degrees]	K_11
0	100
0	100
0	100
0	100
0	100

8. sink(-) /source (+) term per layer:

   0

   0

   0

   0

   0

9. Initial condition is a constant pressure head of -200 cm across the soil.

init. cond [real]	type of init. cond	RCZA method [y/n]	RCZA method val.
0.0	H_tot	n	0
0.0	H_tot	n	0
0.0	H_tot	n	0
0.0	H_tot	n	0
0.0	H_tot	n	0

10. number of boundaries: 2

11.

boundary ID	boundary type	use rain.dat [y/n]	value
101	1	n	0.0
102	2	n	0.5

12. Save matrix.conf.

Contaminant transport *ADE.conf*

1. Open *ADE.conf* in a text editor of your choice.

2. specify coupling with Richards equation [y/n]: y

3. use sorption: n

4. Save ADE.conf.

contaminant.conf

1. Open *contaminant.conf* in a text editor of your choice.

2. number of layers: 5

3. molecular diffusion:

   10e-3

   10e-3

   10e-3

   10e-3

   10e-3

4. dispersivity:

angle [degrees]	D_11
0	30
0	30
0	30
0	30
0	30

5. initial condition:

value	type
0	ca
0	ca
0	ca
2	ca
0	ca

6. number of different orders of reactions: 1

7. orders of reaction:

   1

1

1

1

1

8. reaction coefficients:

   0

   0

   0

   0

   0

9. number of boundaries: 2

10.

boundary ID	boundary type	use rain.dat [y/n]	value
101	1	n	0.0
102	2	n	0.0

11. save *contaminant.conf*

Run scenario 1

Run the simulation in the terminal console.

1. Make sure you are in the right directory.

2. To execute *DRUtES*:

   $ bin/drutes

3. After the simulation finishes, to generate png plots execute provided R script:

   $ Rscript drutes.conf/makeplot.R -name coupled_samesoil

4. The output of the simulation can be found in the folder out

Scenario 2

In scenario 2 we introduce a clay layer in depth 170-180 cm. For this, we need to change matrix.conf and contaminant.conf.

Changes in matrix.conf

1. Change the 2nd van Genuchten parameter set:

alpha	n	m	theta_r	theta_s	specific storage
0.05	2	0.5	0.05	0.45	0
0.01	1.4	0.2857	0.05	0.45	0
0.05	2	0.5	0.05	0.45	0
0.05	2	0.5	0.05	0.45	0
0.05	2	0.5	0.05	0.45	0

2. Change the 2nd hydraulic conductivity. The angle of the anisotropy determines the angle of the reference coordinate system. 0 means vertical flow. Anisotropy description. Anisotpropy description and hydraulic conductivity

angle [degrees]	K_11
0	100
0	1
0	100
0	100
0	100

3. save *matrix.conf*

Changes in contaminant.conf

1. Change the second dispersivity value to 100. dispersivity:

angle [degrees]	D_11
0	30
0	100
0	30
0	30
0	30

2. save contaminant.conf

Run scenario 2

Run the simulation in the terminal console.

1. Make sure you are in the right directory.
2. To execute *DRUtES*:
   $ bin/drutes
3. After the simulation finishes, to generate png plots execute provided R script:
   $ Rscript drutes.conf/makeplot.R -name coupled_claylense
4. The output of the simulation can be found in the folder out

Tasks

1. Describe the distribution of the contaminant without and with the clay layer.
2. Investigate how the simulation differs: (i) With a different soil material (ii) when you include a reaction in contaminant.conf

Simulation Results

The simulation nicely shows how the contamination moves downwards into the soil and disperses to compensate for concentration differences. The clay layer hinders the water flow into deeper layers and therefore also the advection. Due to the high dispersion in the clay layer the contaminant concentration becomes more evenly distributed in that layer.

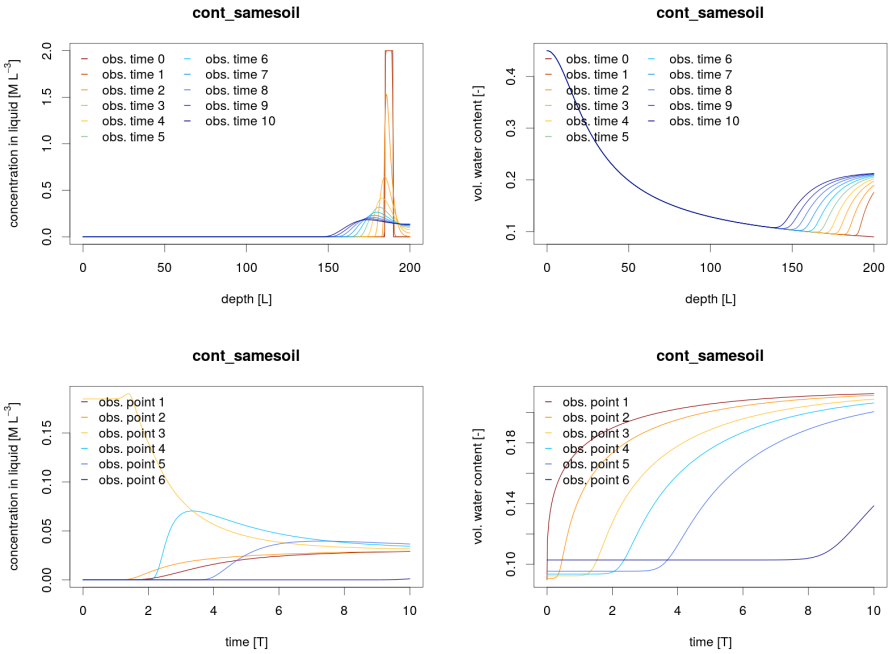


Figure 4.9: Water content and contaminant concentration at the observation points and observation times the homogeneous soil.

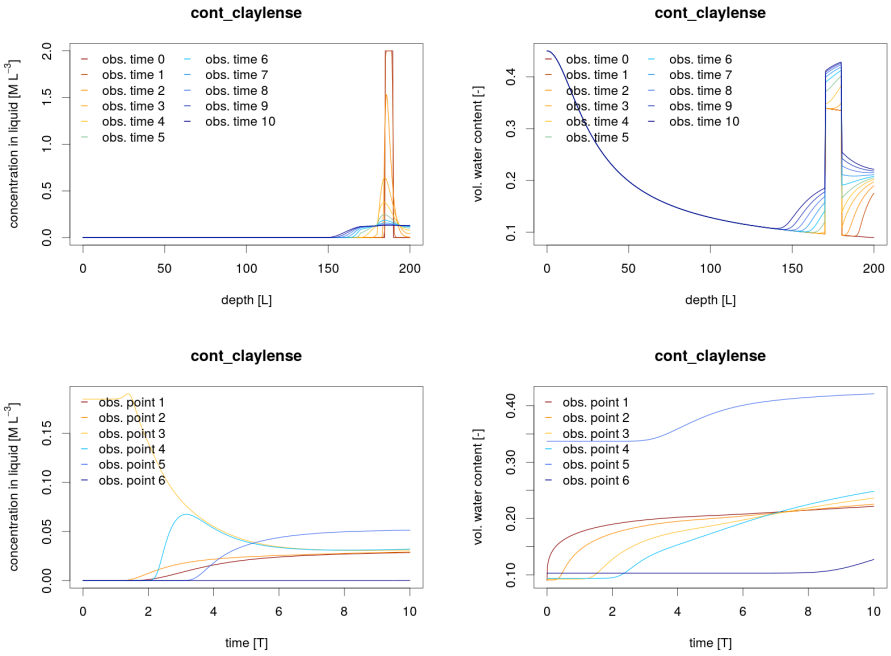


Figure 4.10: Water content and contaminant concentration at the observation points and observation times with a clay layer.

4.2.3 Outcome

1. You got familiar with simple contaminant transport.

2. You simulated coupled water flow and contamination transport.

3. You understand the difference between advection and dispersion.