DRUtES

TUTORIAL: INFILTRATION – PART 1

October 31, 2017

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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

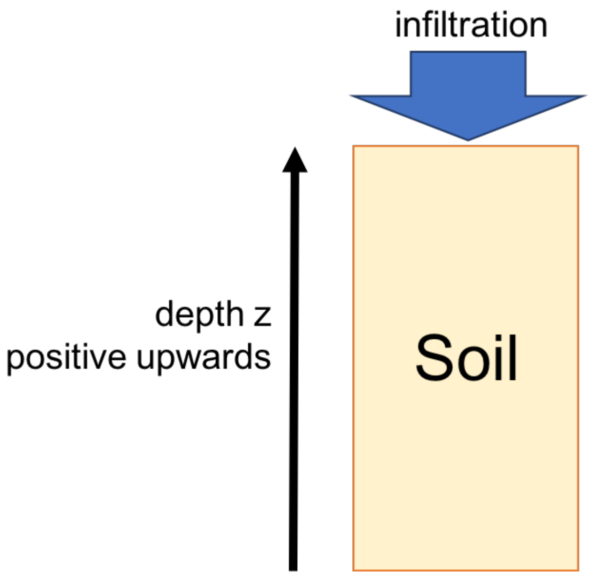

Figure 1: Simplified scheme of infiltration.

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.

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)

SCENARIOS

We are using the well-known van Genuchten-Mualem parameterization to describe the soil hydraulic properties of our soils.

Table 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	0	0	0
K_s [cm d^{-1}]	saturated hydraulic conductivity	400	40	4

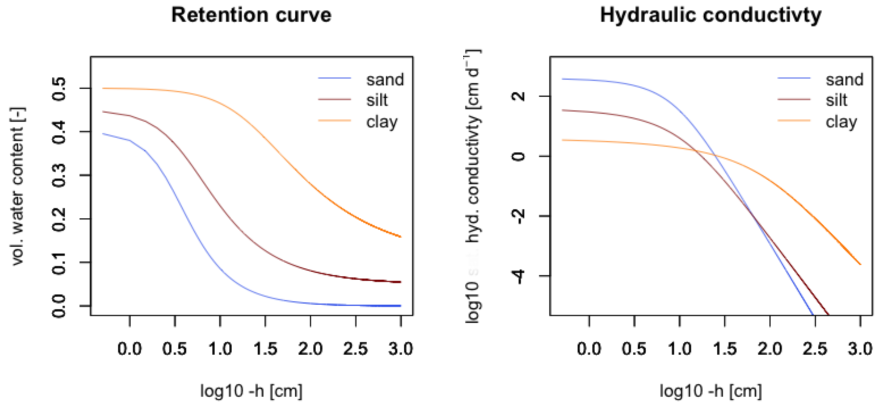

Figure 2: Retention curve and hydraulic conductivity for parameterized with van Genuchten model for sand, silt and clay.

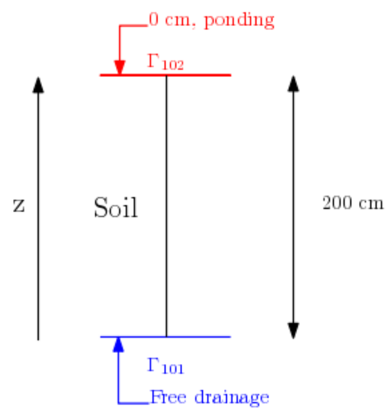

Figure 3: 1D domain set-up of infiltration scenario with top and bottom boundary conditions. A constant ponding is assigned to the top, defined with a Dirichlet condition of 0 cm. Free drainage occurs at the bottom, which indicates that the pressure head gradient is 0 and water flows only due to gravity.

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*

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
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).

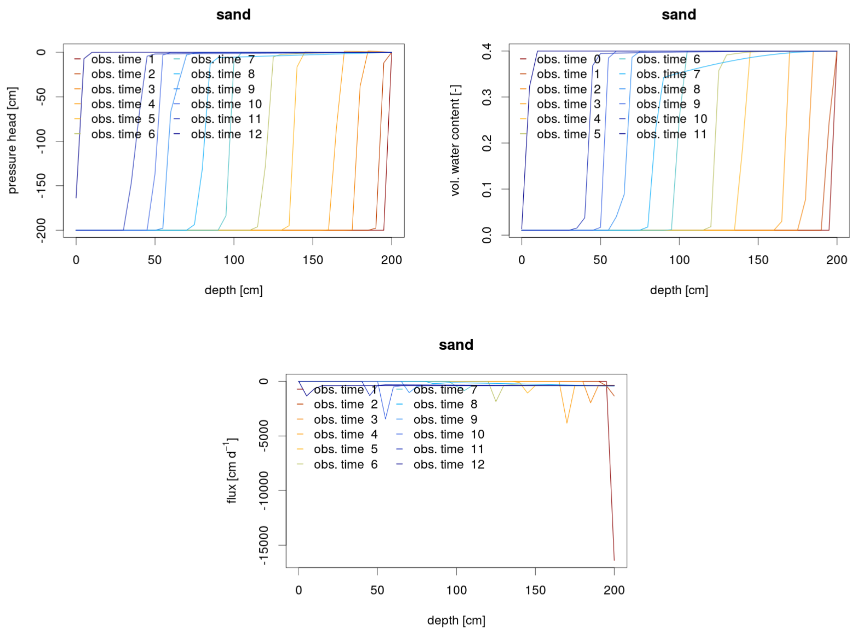

Figure 4: Observation time series of pressure head, vol. water content and flux of infiltration into sand.

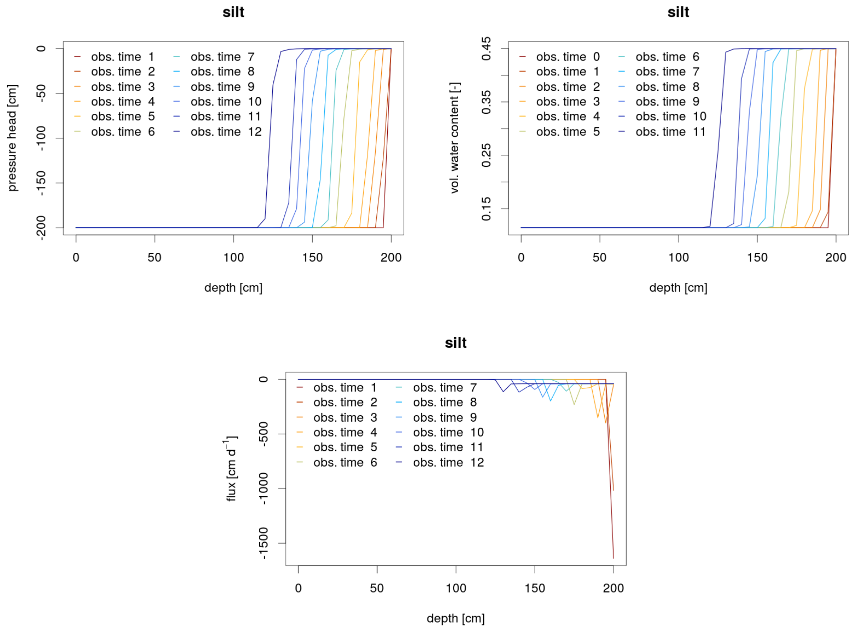

Figure 5: Observation time series of pressure head, vol. water content and flux of infiltration into silt.

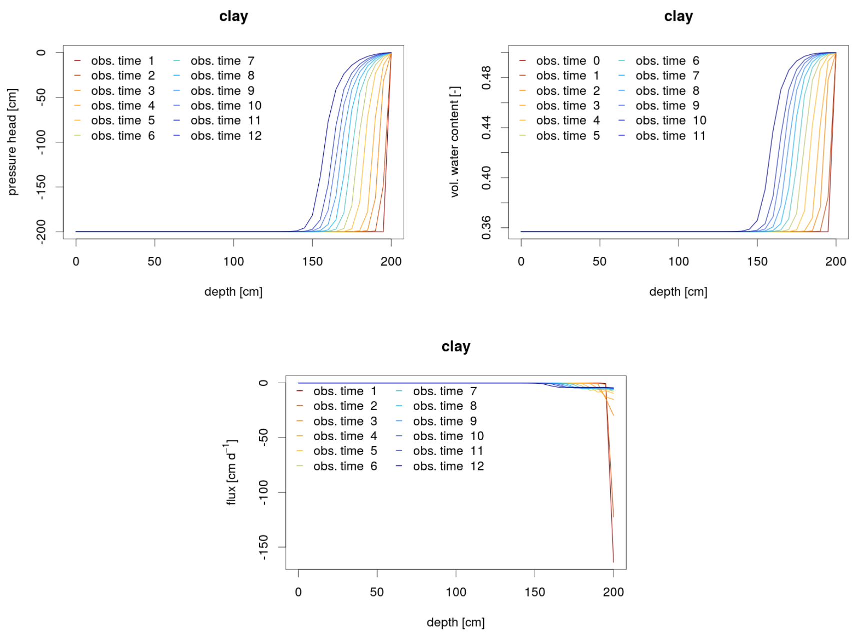

Figure 6: Observation time series of pressure head, vol. water content and flux of infiltration into clay.

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.

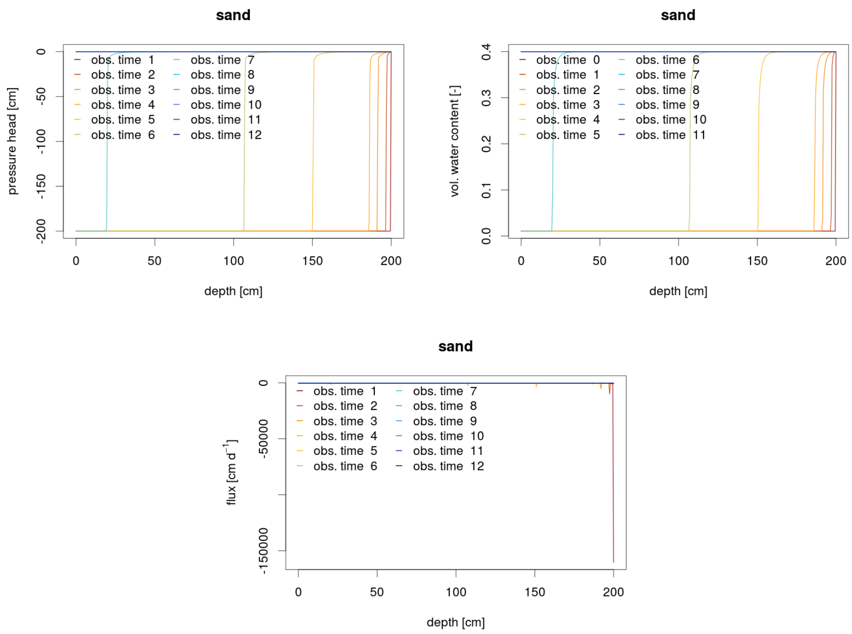

Figure 7: Observation time series of pressure head, vol. water content and flux of infiltration into sand with improved discretization.

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.

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.